



Full wwPDB EM Validation Report (i)

Dec 12, 2022 – 03:07 am GMT

PDB ID : 5A1Y
EMDB ID : EMD-2989
Title : The structure of the COPI coat linkage IV
Authors : Dodonova, S.O.; Diestelkoetter-Bachert, P.; von Appen, A.; Hagen, W.J.H.; Beck, R.; Beck, M.; Wieland, F.; Briggs, J.A.G.
Deposited on : 2015-05-06
Resolution : 21.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references \(i\)](#)) were used in the production of this report:

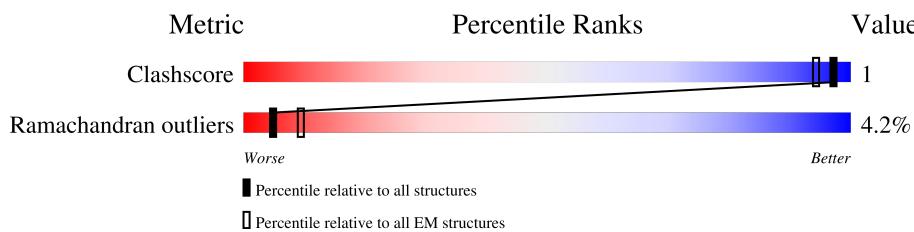
EMDB validation analysis : 0.0.1.dev43
MolProbit : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

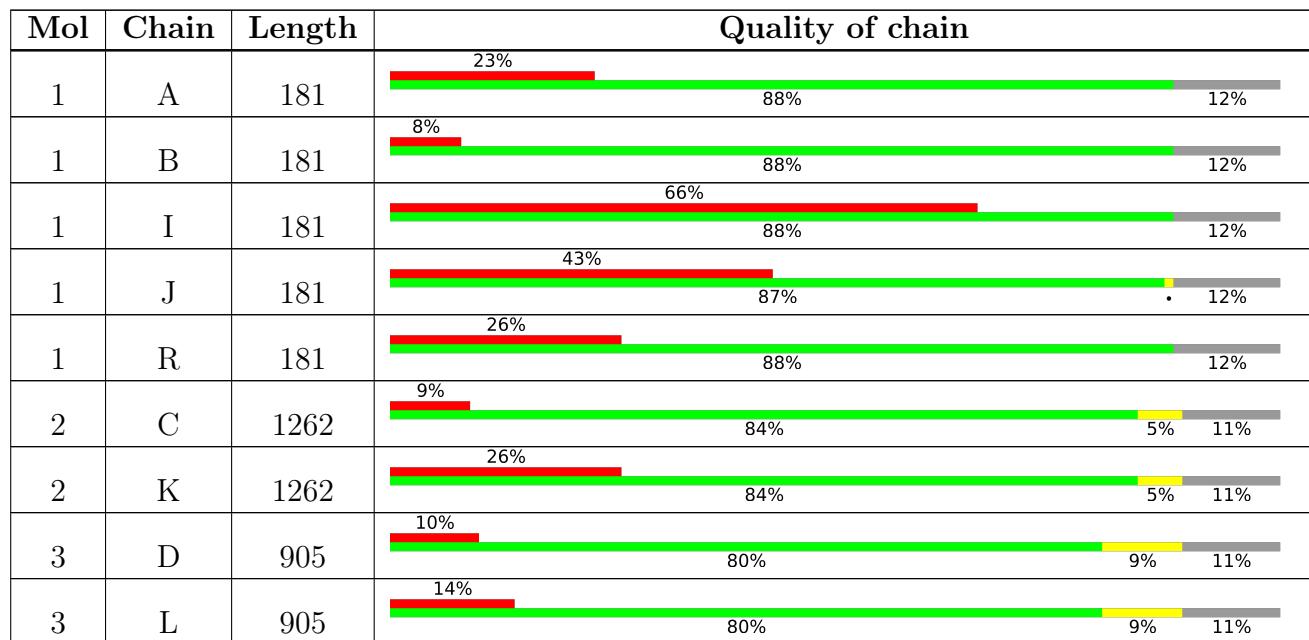
The reported resolution of this entry is 21.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



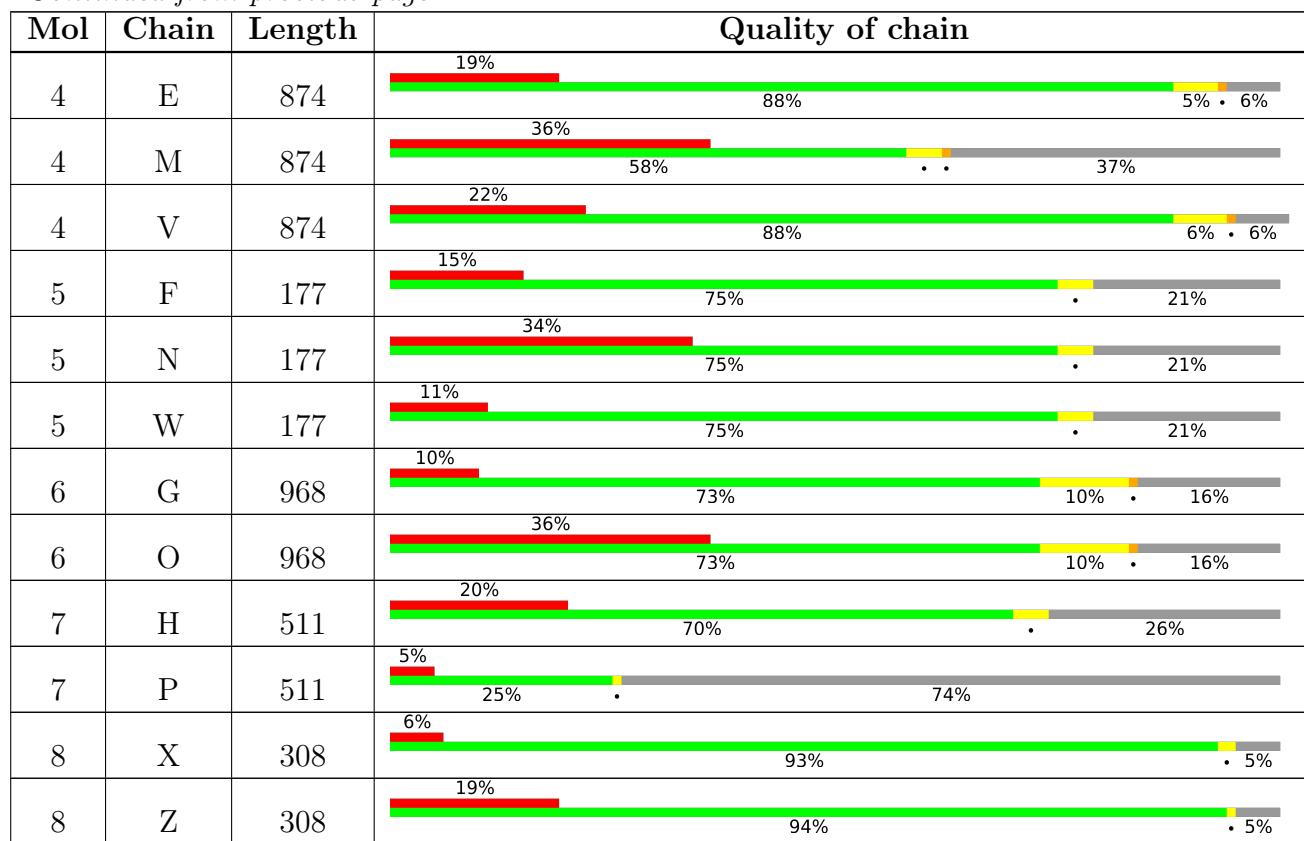
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.



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2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 39957 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ADP-RIBOSYLATION FACTOR 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	159	Total 636	C 318	N 159	O 159	0	0
1	B	159	Total 636	C 318	N 159	O 159	0	0
1	I	159	Total 636	C 318	N 159	O 159	0	0
1	J	159	Total 636	C 318	N 159	O 159	0	0
1	R	159	Total 636	C 318	N 159	O 159	0	0

- Molecule 2 is a protein called COATOMER SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	1126	Total 4503	C 2252	N 1126	O 1125	0	0
2	K	1126	Total 4503	C 2252	N 1126	O 1125	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1225	LEU	-	expression tag	UNP Q8CIE6
C	1226	GLU	-	expression tag	UNP Q8CIE6
C	1227	VAL	-	expression tag	UNP Q8CIE6
C	1228	LEU	-	expression tag	UNP Q8CIE6
C	1229	PHE	-	expression tag	UNP Q8CIE6
C	1230	GLN	-	expression tag	UNP Q8CIE6
C	1231	GLY	-	expression tag	UNP Q8CIE6
C	1232	PRO	-	expression tag	UNP Q8CIE6
C	1233	SER	-	expression tag	UNP Q8CIE6
C	1234	ALA	-	expression tag	UNP Q8CIE6
C	1235	TRP	-	expression tag	UNP Q8CIE6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1236	SER	-	expression tag	UNP Q8CIE6
C	1237	HIS	-	expression tag	UNP Q8CIE6
C	1238	PRO	-	expression tag	UNP Q8CIE6
C	1239	GLN	-	expression tag	UNP Q8CIE6
C	1240	PHE	-	expression tag	UNP Q8CIE6
C	1241	GLU	-	expression tag	UNP Q8CIE6
C	1242	LYS	-	expression tag	UNP Q8CIE6
C	1243	GLY	-	expression tag	UNP Q8CIE6
C	1244	GLY	-	expression tag	UNP Q8CIE6
C	1245	GLY	-	expression tag	UNP Q8CIE6
C	1246	SER	-	expression tag	UNP Q8CIE6
C	1247	GLY	-	expression tag	UNP Q8CIE6
C	1248	GLY	-	expression tag	UNP Q8CIE6
C	1249	GLY	-	expression tag	UNP Q8CIE6
C	1250	SER	-	expression tag	UNP Q8CIE6
C	1251	GLY	-	expression tag	UNP Q8CIE6
C	1252	GLY	-	expression tag	UNP Q8CIE6
C	1253	SER	-	expression tag	UNP Q8CIE6
C	1254	ALA	-	expression tag	UNP Q8CIE6
C	1255	TRP	-	expression tag	UNP Q8CIE6
C	1256	SER	-	expression tag	UNP Q8CIE6
C	1257	HIS	-	expression tag	UNP Q8CIE6
C	1258	PRO	-	expression tag	UNP Q8CIE6
C	1259	GLN	-	expression tag	UNP Q8CIE6
C	1260	PHE	-	expression tag	UNP Q8CIE6
C	1261	GLU	-	expression tag	UNP Q8CIE6
C	1262	LYS	-	expression tag	UNP Q8CIE6
K	1225	LEU	-	expression tag	UNP Q8CIE6
K	1226	GLU	-	expression tag	UNP Q8CIE6
K	1227	VAL	-	expression tag	UNP Q8CIE6
K	1228	LEU	-	expression tag	UNP Q8CIE6
K	1229	PHE	-	expression tag	UNP Q8CIE6
K	1230	GLN	-	expression tag	UNP Q8CIE6
K	1231	GLY	-	expression tag	UNP Q8CIE6
K	1232	PRO	-	expression tag	UNP Q8CIE6
K	1233	SER	-	expression tag	UNP Q8CIE6
K	1234	ALA	-	expression tag	UNP Q8CIE6
K	1235	TRP	-	expression tag	UNP Q8CIE6
K	1236	SER	-	expression tag	UNP Q8CIE6
K	1237	HIS	-	expression tag	UNP Q8CIE6
K	1238	PRO	-	expression tag	UNP Q8CIE6
K	1239	GLN	-	expression tag	UNP Q8CIE6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1240	PHE	-	expression tag	UNP Q8CIE6
K	1241	GLU	-	expression tag	UNP Q8CIE6
K	1242	LYS	-	expression tag	UNP Q8CIE6
K	1243	GLY	-	expression tag	UNP Q8CIE6
K	1244	GLY	-	expression tag	UNP Q8CIE6
K	1245	GLY	-	expression tag	UNP Q8CIE6
K	1246	SER	-	expression tag	UNP Q8CIE6
K	1247	GLY	-	expression tag	UNP Q8CIE6
K	1248	GLY	-	expression tag	UNP Q8CIE6
K	1249	GLY	-	expression tag	UNP Q8CIE6
K	1250	SER	-	expression tag	UNP Q8CIE6
K	1251	GLY	-	expression tag	UNP Q8CIE6
K	1252	GLY	-	expression tag	UNP Q8CIE6
K	1253	SER	-	expression tag	UNP Q8CIE6
K	1254	ALA	-	expression tag	UNP Q8CIE6
K	1255	TRP	-	expression tag	UNP Q8CIE6
K	1256	SER	-	expression tag	UNP Q8CIE6
K	1257	HIS	-	expression tag	UNP Q8CIE6
K	1258	PRO	-	expression tag	UNP Q8CIE6
K	1259	GLN	-	expression tag	UNP Q8CIE6
K	1260	PHE	-	expression tag	UNP Q8CIE6
K	1261	GLU	-	expression tag	UNP Q8CIE6
K	1262	LYS	-	expression tag	UNP Q8CIE6

- Molecule 3 is a protein called COATOMER SUBUNIT BETA'.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	D	803	Total C N O 3211 1606 803 802	0	0
3	L	803	Total C N O 3211 1606 803 802	0	0

- Molecule 4 is a protein called COATOMER SUBUNIT GAMMA-1.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	E	824	Total C N O 3294 1648 824 822	0	0
4	M	550	Total C N O 2199 1100 550 549	0	0
4	V	824	Total C N O 3294 1648 824 822	0	0

- Molecule 5 is a protein called COATOMER SUBUNIT ZETA-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	139	Total	C	N	O		
			555	278	139	138	0	0
5	N	139	Total	C	N	O		
			555	278	139	138	0	0
5	W	139	Total	C	N	O		
			555	278	139	138	0	0

- Molecule 6 is a protein called COATOMER SUBUNIT BETA.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	813	Total	C	N	O		
			3250	1626	813	811	0	0
6	O	813	Total	C	N	O		
			3250	1626	813	811	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	MET	-	expression tag	UNP Q9JIF7
G	-13	HIS	-	expression tag	UNP Q9JIF7
G	-12	HIS	-	expression tag	UNP Q9JIF7
G	-11	HIS	-	expression tag	UNP Q9JIF7
G	-10	HIS	-	expression tag	UNP Q9JIF7
G	-9	HIS	-	expression tag	UNP Q9JIF7
G	-8	HIS	-	expression tag	UNP Q9JIF7
G	-7	GLU	-	expression tag	UNP Q9JIF7
G	-6	ASN	-	expression tag	UNP Q9JIF7
G	-5	LEU	-	expression tag	UNP Q9JIF7
G	-4	TYR	-	expression tag	UNP Q9JIF7
G	-3	PHE	-	expression tag	UNP Q9JIF7
G	-2	GLN	-	expression tag	UNP Q9JIF7
G	-1	GLY	-	expression tag	UNP Q9JIF7
G	0	HIS	-	expression tag	UNP Q9JIF7
O	-14	MET	-	expression tag	UNP Q9JIF7
O	-13	HIS	-	expression tag	UNP Q9JIF7
O	-12	HIS	-	expression tag	UNP Q9JIF7
O	-11	HIS	-	expression tag	UNP Q9JIF7
O	-10	HIS	-	expression tag	UNP Q9JIF7
O	-9	HIS	-	expression tag	UNP Q9JIF7
O	-8	HIS	-	expression tag	UNP Q9JIF7
O	-7	GLU	-	expression tag	UNP Q9JIF7

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-6	ASN	-	expression tag	UNP Q9JIF7
O	-5	LEU	-	expression tag	UNP Q9JIF7
O	-4	TYR	-	expression tag	UNP Q9JIF7
O	-3	PHE	-	expression tag	UNP Q9JIF7
O	-2	GLN	-	expression tag	UNP Q9JIF7
O	-1	GLY	-	expression tag	UNP Q9JIF7
O	0	HIS	-	expression tag	UNP Q9JIF7

- Molecule 7 is a protein called COATOMER SUBUNIT DELTA.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	H	380	Total C N O 1520 760 380 380	0	0
7	P	135	Total C N O 539 270 135 134	0	0

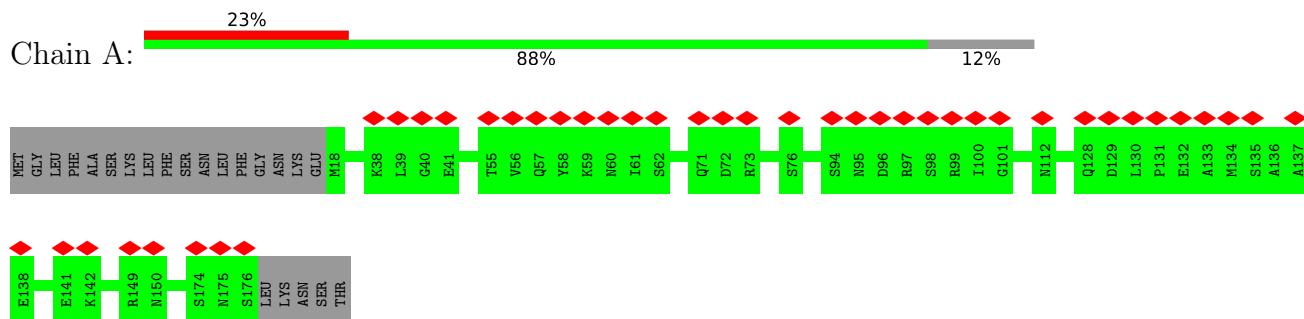
- Molecule 8 is a protein called COATOMER SUBUNIT EPSILON.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	X	292	Total C N O 1169 584 292 293	0	0
8	Z	292	Total C N O 1169 584 292 293	0	0

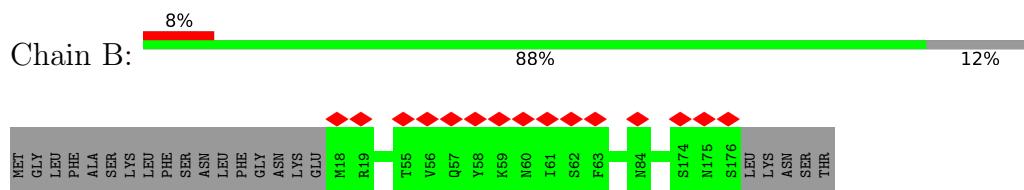
3 Residue-property plots [\(i\)](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

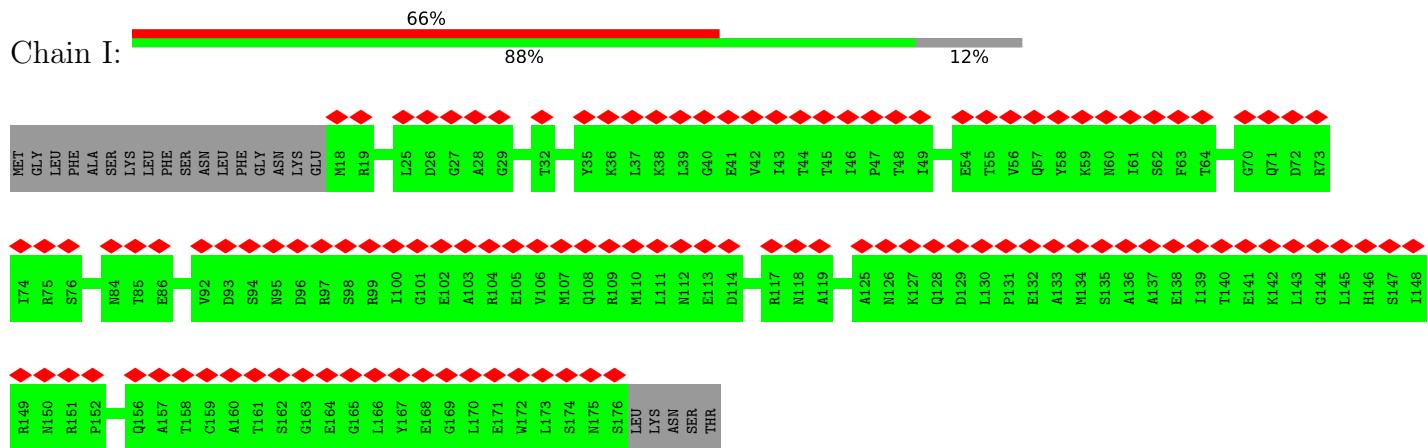
- Molecule 1: ADP-RIBOSYLATION FACTOR 1



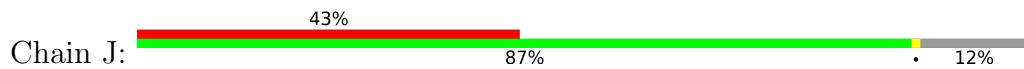
- Molecule 1: ADP-RIBOSYLATION FACTOR 1

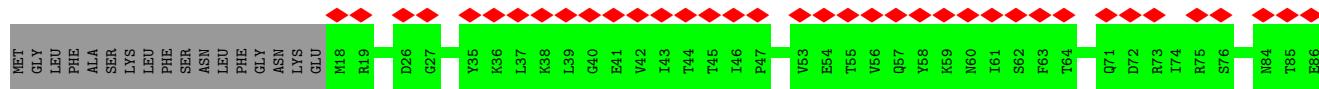


- Molecule 1: ADP-RIBOSYLATION FACTOR 1

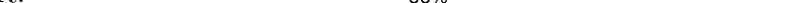


- Molecule 1: ADP-RIBOSYLATION FACTOR 1



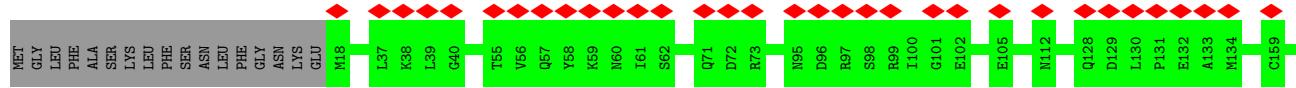


- Molecule 1: ADP-RIBOSYLATION FACTOR 1



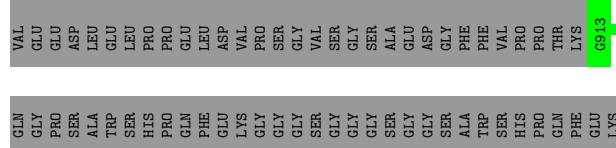
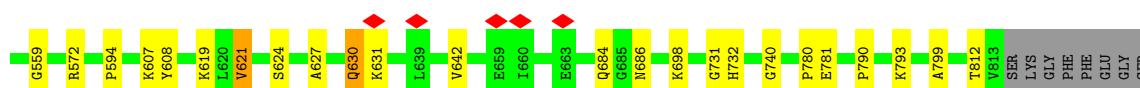
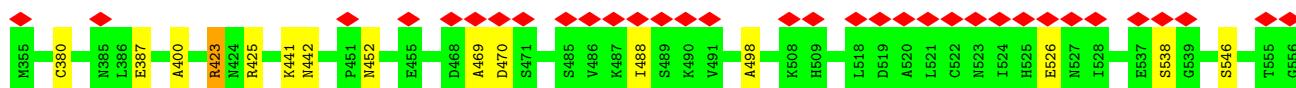
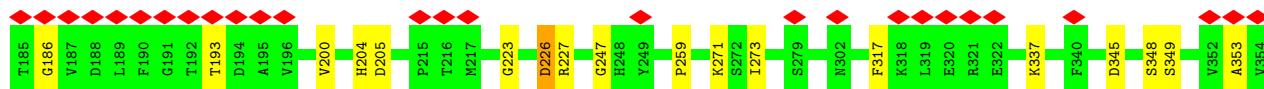
Chain R: 26% 88% 12%

A horizontal bar chart with three bars. The first bar is red and labeled '26%'. The second bar is green and labeled '88%'. The third bar is blue and labeled '12%'. The bars are positioned side-by-side, representing the proportion of Chain R in each category.



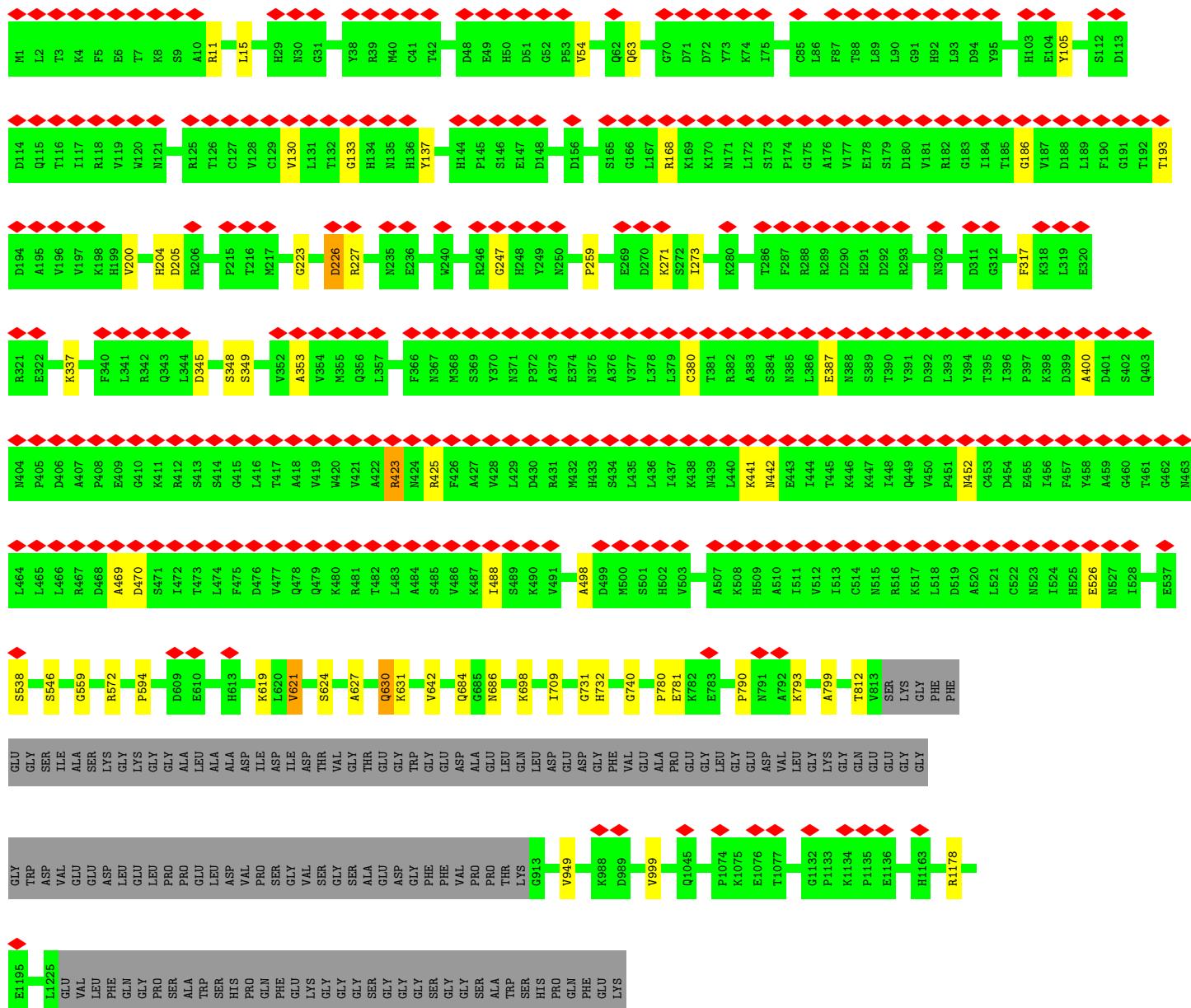
- Molecule 2: COATOMER SUBUNIT ALPHA

Category	Percentage
Red	9%
Green	84%
Blue	5%
Yellow	11%



- Molecule 2: COATOMER SUBUNIT ALPHA

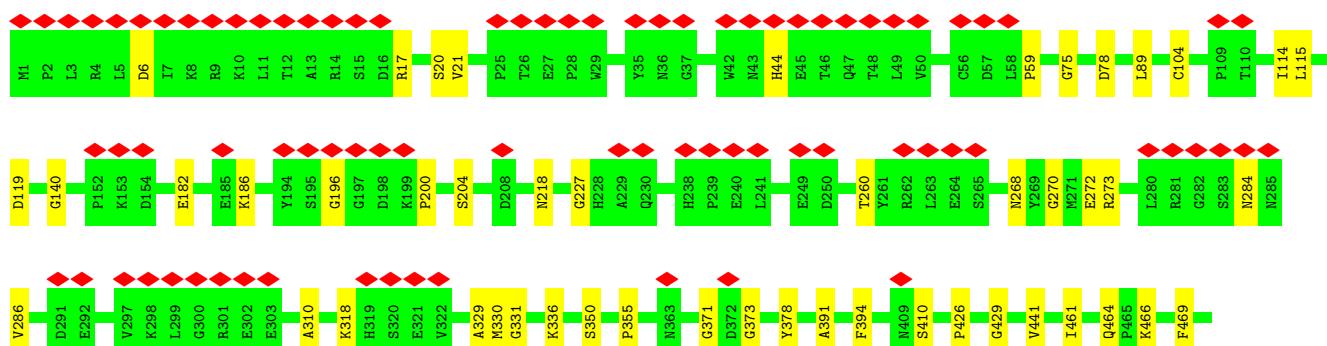
A horizontal bar chart illustrating the distribution of Chain K. The x-axis represents the total length of Chain K, which is 100% (indicated by the 11% label at the end of the bar). The bar is divided into four segments: a red segment at the beginning labeled 26%, a long green segment labeled 84% in the center, a small yellow segment labeled 5% near the end, and a grey segment labeled 11% at the far right.

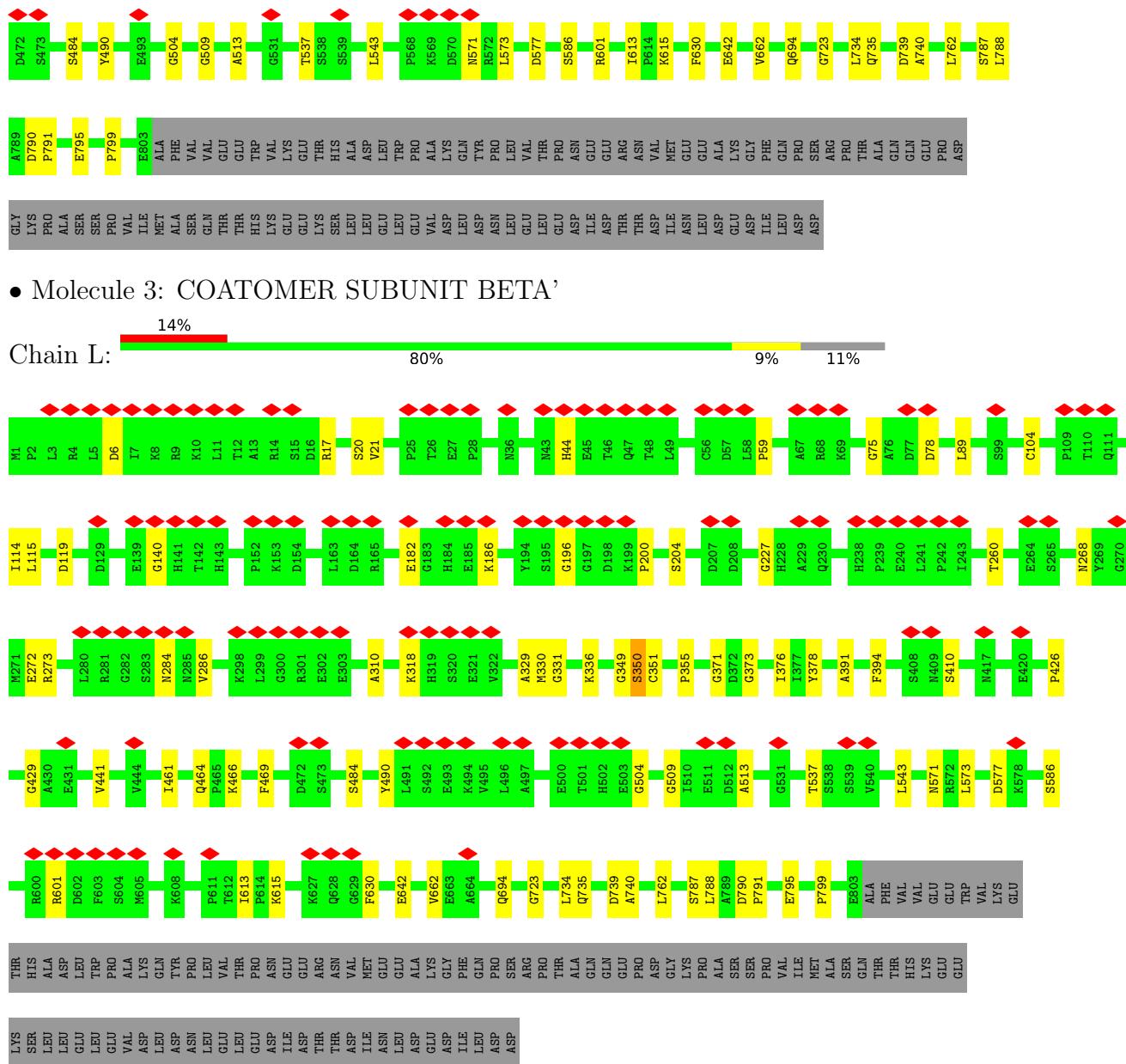


- Molecule 3: COATOMER SUBUNIT BETA'

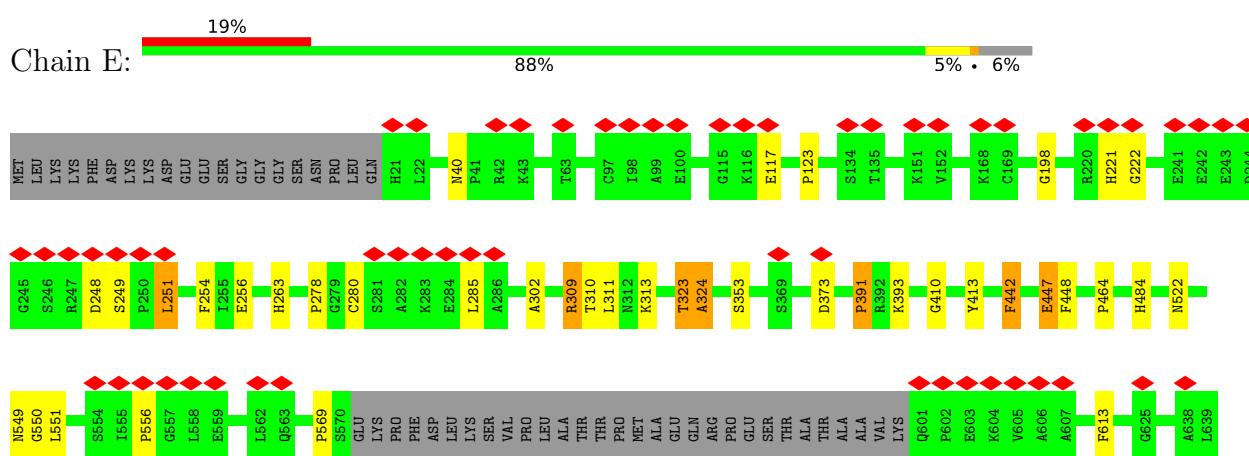
A horizontal bar chart titled "Chain D" showing its distribution across four categories. The categories are represented by colored segments: red (10%), green (80%), yellow (9%), and grey (11%).

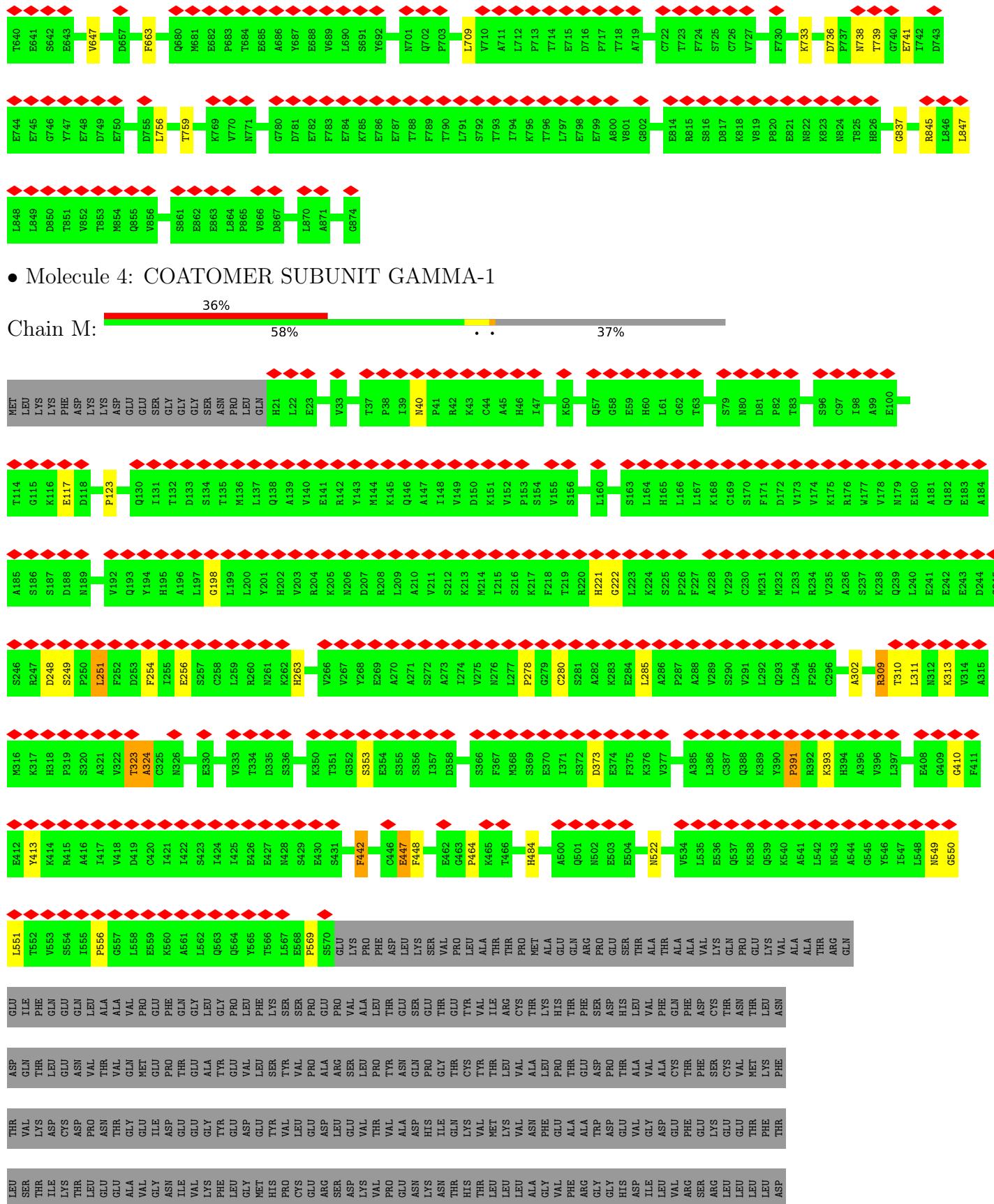
Category	Percentage
Red	10%
Green	80%
Yellow	9%
Grey	11%





- Molecule 4: COATOMER SUBUNIT GAMMA-1

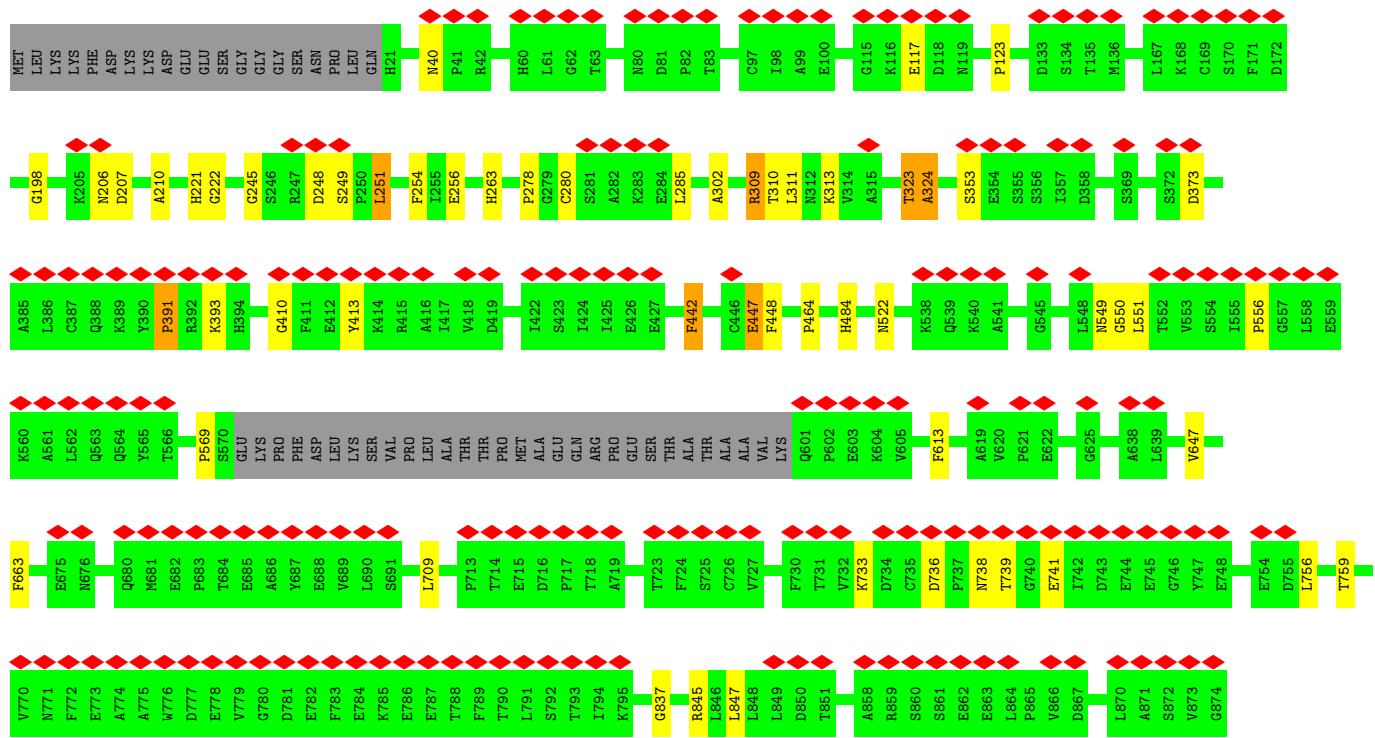




- Molecule 4: COATOMER SUBUNIT GAMMA-1

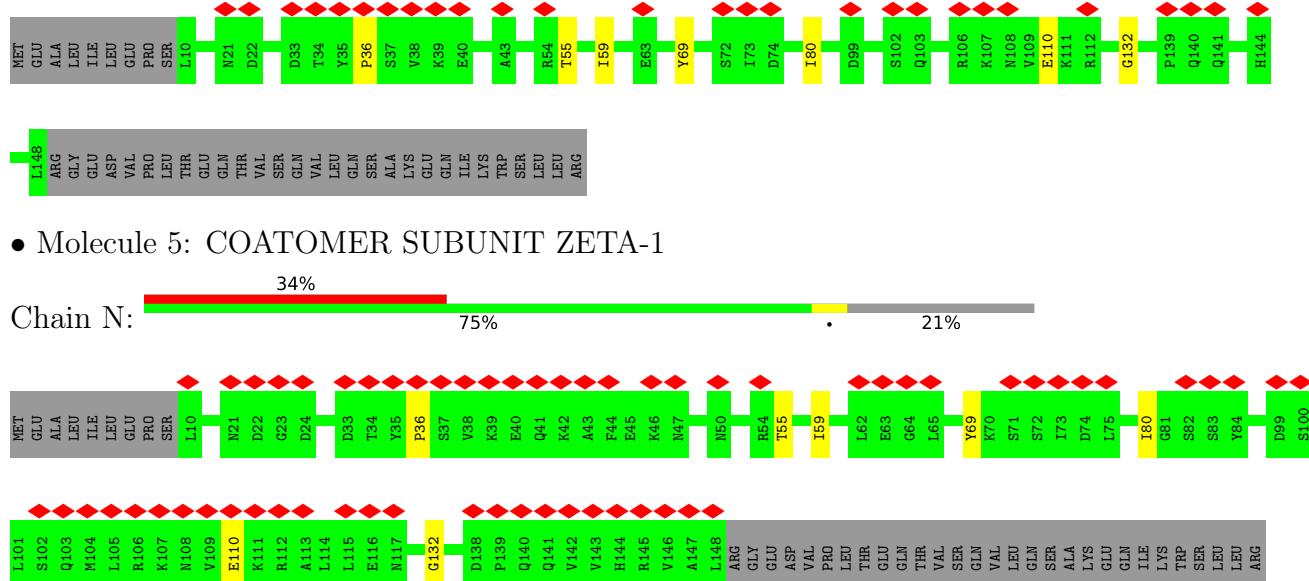
A horizontal bar chart illustrating the composition of Chain V. The total length of the bar is 100%, divided into three segments: a red segment at 22%, a green segment at 88%, and a yellow segment at 6%.

Component	Percentage
Red	22%
Green	88%
Yellow	6%

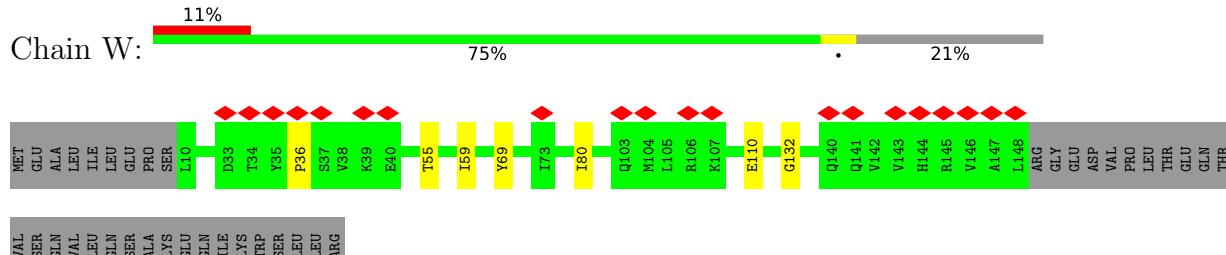


- Molecule 5: COATOMER SUBUNIT ZETA-1

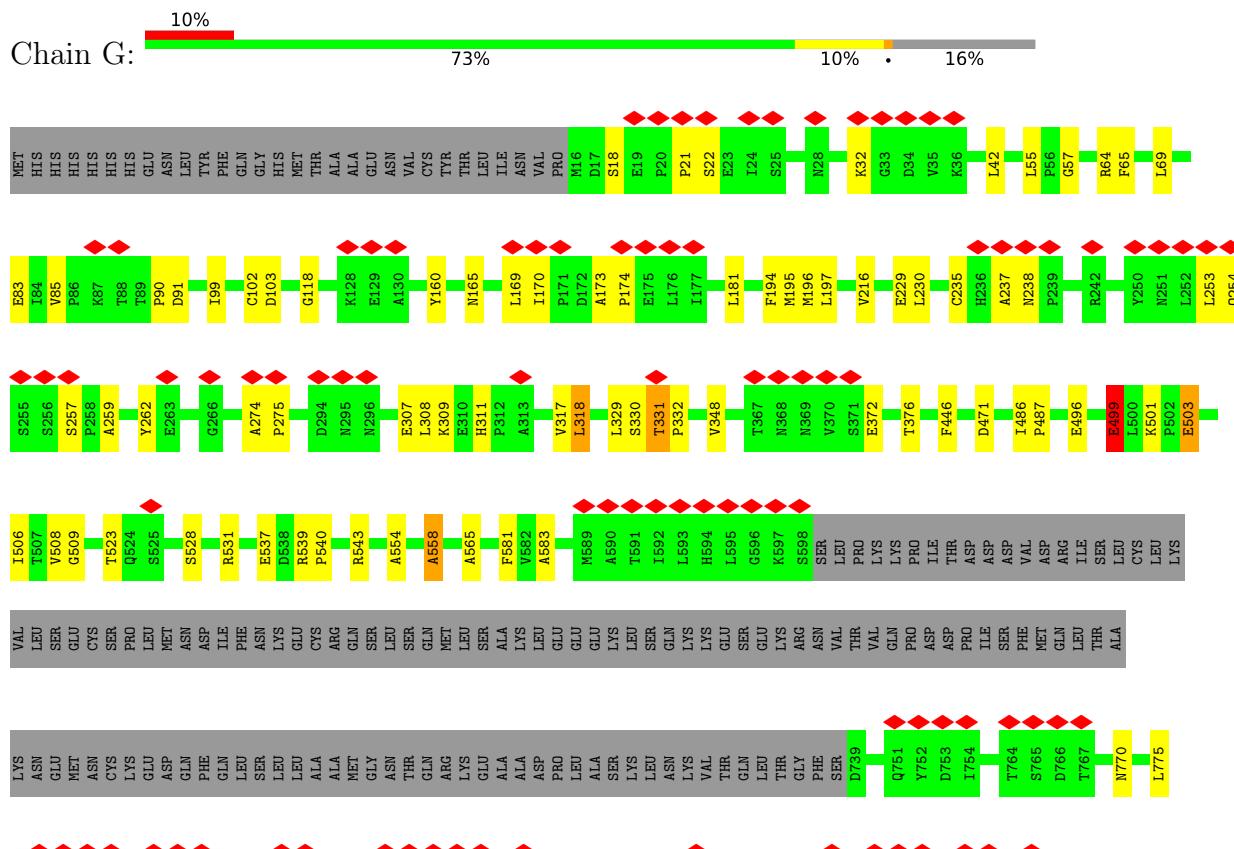
Chain F: 15% • 75% • 21%



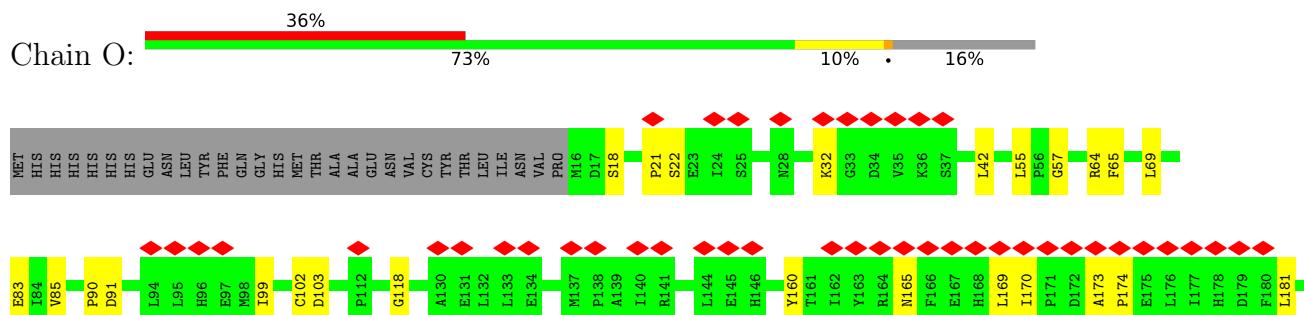
- Molecule 5: COATOMER SUBUNIT ZETA-1

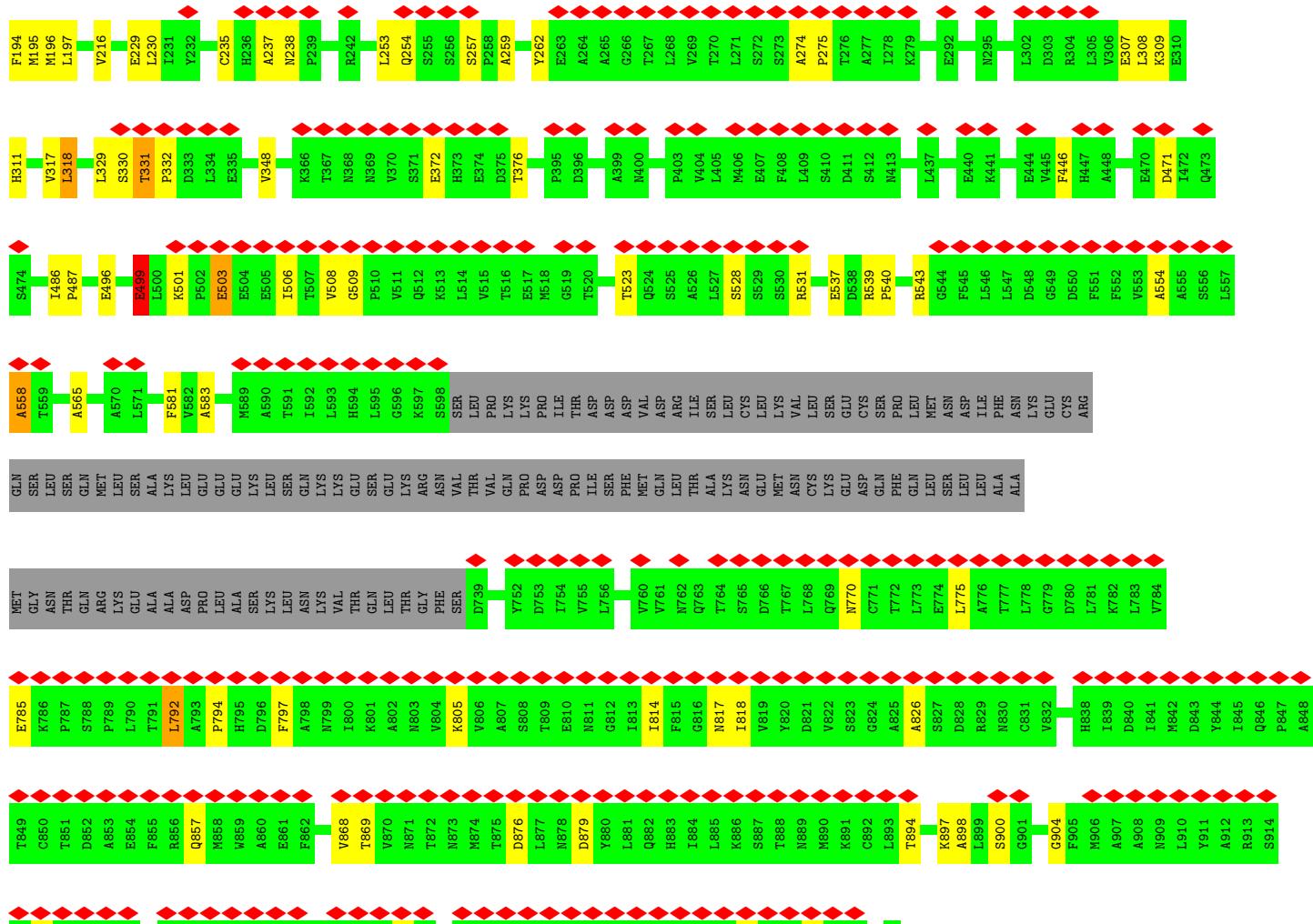


- Molecule 6: COATOMER SUBUNIT BETA

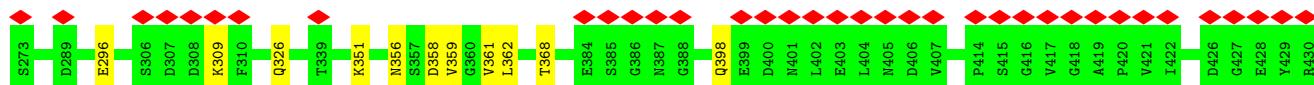


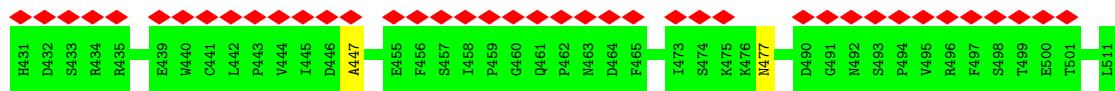
- Molecule 6: COATOMER SUBUNIT BETA





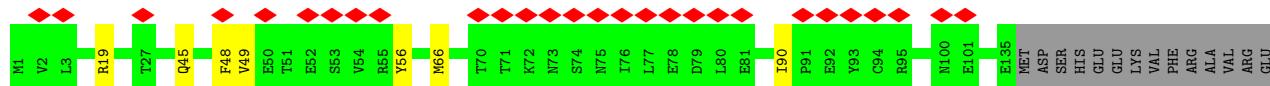
- Molecule 7: COATOMER SUBUNIT DELTA





• Molecule 7: COATOMER SUBUNIT DELTA

Chain P: 5% 25% • 74%



• Molecule 8: COATOMER SUBUNIT EPSILON

Chain X: 6% 93% • 5%



• Molecule 8: COATOMER SUBUNIT EPSILON

Chain X: 6% 93% • 5%



• Molecule 8: COATOMER SUBUNIT EPSILON

Chain Z: 19% 94% • 5%



4 Experimental information i

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of tilted images used	1205	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING OF INDIVIDUAL TILTS	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	42000	Depositor
Image detector	GATAN MULTISCAN	Depositor
Maximum voxel value	6.961	Depositor
Minimum voxel value	-5.585	Depositor
Average voxel value	0.033	Depositor
Voxel value standard deviation	0.924	Depositor
Recommended contour level	1.5	Depositor
Tomogram size (Å)	403.80002, 403.80002, 403.80002	wwPDB
Tomogram dimensions	200, 200, 200	wwPDB
Tomogram angles (°)	90.0, 90.0, 90.0	wwPDB
Grid spacing (Å)	2.019, 2.019, 2.019	Depositor

5 Model quality i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	0/635	0.69	0/792
1	B	0.43	0/635	0.69	0/792
1	I	0.43	0/635	0.69	0/792
1	J	0.43	0/635	0.69	0/792
1	R	0.43	0/635	0.69	0/792
2	C	1.40	8/4501 (0.2%)	1.50	13/5623 (0.2%)
2	K	1.40	8/4501 (0.2%)	1.50	14/5623 (0.2%)
3	D	1.60	16/3210 (0.5%)	1.72	24/4011 (0.6%)
3	L	1.60	16/3210 (0.5%)	1.72	23/4011 (0.6%)
4	E	1.52	4/3292 (0.1%)	1.63	19/4112 (0.5%)
4	M	1.52	2/2198 (0.1%)	1.58	9/2746 (0.3%)
4	V	1.52	4/3292 (0.1%)	1.63	19/4112 (0.5%)
5	F	1.55	1/554 (0.2%)	1.74	3/691 (0.4%)
5	N	1.55	1/554 (0.2%)	1.74	3/691 (0.4%)
5	W	1.55	1/554 (0.2%)	1.74	3/691 (0.4%)
6	G	1.50	7/3248 (0.2%)	1.71	23/4057 (0.6%)
6	O	1.50	7/3248 (0.2%)	1.71	23/4057 (0.6%)
7	H	1.21	0/1518	1.34	8/1893 (0.4%)
7	P	1.46	0/538	1.76	7/671 (1.0%)
8	X	0.91	0/1168	0.63	0/1457
8	Z	0.91	0/1168	0.63	0/1457
All	All	1.40	75/39929 (0.2%)	1.53	191/49863 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	4
2	K	0	4
3	D	0	2
3	L	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	E	0	4
4	M	0	4
4	V	0	4
5	F	0	1
5	N	0	1
5	W	0	1
6	G	0	14
6	O	0	14
All	All	0	55

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	621	VAL	C-N	6.95	1.45	1.33
2	C	621	VAL	C-N	6.95	1.45	1.33
3	D	330	MET	N-CA	-6.82	1.32	1.46
3	L	330	MET	N-CA	-6.80	1.32	1.46
4	V	198	GLY	CA-C	-6.48	1.41	1.51
4	E	198	GLY	CA-C	-6.46	1.41	1.51
4	M	198	GLY	CA-C	-6.43	1.41	1.51
3	L	378	TYR	N-CA	-6.37	1.33	1.46
3	D	537	THR	N-CA	-6.37	1.33	1.46
3	L	537	THR	N-CA	-6.36	1.33	1.46
3	D	378	TYR	N-CA	-6.35	1.33	1.46
6	O	118	GLY	CA-C	-6.32	1.41	1.51
3	L	723	GLY	CA-C	-6.29	1.41	1.51
3	D	723	GLY	CA-C	-6.27	1.41	1.51
6	G	118	GLY	CA-C	-6.27	1.41	1.51
3	L	799	PRO	C-N	6.23	1.44	1.33
3	D	799	PRO	C-N	6.19	1.44	1.33
3	D	464	GLN	N-CA	-6.13	1.34	1.46
3	L	464	GLN	N-CA	-6.10	1.34	1.46
4	E	123	PRO	N-CA	-6.00	1.37	1.47
3	L	186	LYS	C-N	5.96	1.43	1.33
4	V	123	PRO	N-CA	-5.95	1.37	1.47
4	M	123	PRO	N-CA	-5.92	1.37	1.47
3	D	186	LYS	C-N	5.92	1.43	1.33
2	C	631	LYS	N-CA	-5.90	1.34	1.46
3	L	331	GLY	CA-C	-5.90	1.42	1.51
2	K	631	LYS	N-CA	-5.88	1.34	1.46
3	D	331	GLY	CA-C	-5.84	1.42	1.51
2	C	204	HIS	N-CA	-5.79	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	227	GLY	CA-C	-5.76	1.42	1.51
2	K	204	HIS	N-CA	-5.75	1.34	1.46
3	L	373	GLY	N-CA	-5.75	1.37	1.46
3	L	227	GLY	CA-C	-5.72	1.42	1.51
4	E	837	GLY	N-CA	-5.72	1.37	1.46
3	D	373	GLY	N-CA	-5.70	1.37	1.46
4	V	837	GLY	N-CA	-5.67	1.37	1.46
6	O	509	GLY	CA-C	-5.65	1.42	1.51
6	G	509	GLY	CA-C	-5.61	1.42	1.51
2	C	259	PRO	CA-C	-5.46	1.42	1.52
2	K	186	GLY	N-CA	-5.45	1.37	1.46
6	G	539	ARG	C-N	5.43	1.44	1.34
2	K	259	PRO	CA-C	-5.42	1.42	1.52
6	O	539	ARG	C-N	5.41	1.44	1.34
2	C	186	GLY	N-CA	-5.38	1.38	1.46
4	E	613	PHE	N-CA	-5.34	1.35	1.46
5	N	132	GLY	N-CA	-5.33	1.38	1.46
4	V	613	PHE	N-CA	-5.30	1.35	1.46
5	W	132	GLY	N-CA	-5.30	1.38	1.46
5	F	132	GLY	N-CA	-5.28	1.38	1.46
6	O	57	GLY	N-CA	5.26	1.53	1.46
2	K	740	GLY	CA-C	-5.25	1.43	1.51
3	L	466	LYS	N-CA	-5.22	1.35	1.46
6	G	57	GLY	N-CA	5.21	1.53	1.46
6	G	160	TYR	N-CA	-5.20	1.35	1.46
3	D	466	LYS	N-CA	-5.20	1.35	1.46
3	D	509	GLY	N-CA	-5.19	1.38	1.46
2	C	353	ALA	N-CA	-5.19	1.35	1.46
2	K	353	ALA	N-CA	-5.19	1.35	1.46
3	L	310	ALA	N-CA	-5.18	1.35	1.46
2	C	740	GLY	CA-C	-5.17	1.43	1.51
6	O	160	TYR	N-CA	-5.16	1.36	1.46
3	L	504	GLY	N-CA	5.16	1.53	1.46
3	D	310	ALA	N-CA	-5.16	1.36	1.46
2	K	130	VAL	C-N	5.15	1.45	1.34
3	L	586	SER	N-CA	-5.13	1.36	1.46
2	C	130	VAL	C-N	5.13	1.45	1.34
3	L	509	GLY	N-CA	-5.12	1.38	1.46
3	D	504	GLY	N-CA	5.11	1.53	1.46
3	D	586	SER	N-CA	-5.10	1.36	1.46
3	L	371	GLY	CA-C	-5.07	1.43	1.51
6	G	857	GLN	N-CA	-5.06	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	371	GLY	CA-C	-5.06	1.43	1.51
6	O	857	GLN	N-CA	-5.06	1.36	1.46
6	G	565	ALA	N-CA	-5.00	1.36	1.46
6	O	565	ALA	N-CA	-5.00	1.36	1.46

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	496	GLU	N-CA-C	7.83	132.14	111.00
6	G	496	GLU	N-CA-C	7.82	132.12	111.00
4	M	302	ALA	C-N-CA	7.05	139.32	121.70
4	V	302	ALA	C-N-CA	7.04	139.31	121.70
4	E	302	ALA	C-N-CA	7.04	139.29	121.70
2	C	54	VAL	N-CA-C	-6.91	92.35	111.00
2	K	54	VAL	N-CA-C	-6.91	92.34	111.00
6	O	486	ILE	O-C-N	-6.79	108.20	121.10
6	G	486	ILE	O-C-N	-6.78	108.21	121.10
6	G	869	THR	N-CA-C	-6.73	92.83	111.00
6	O	869	THR	N-CA-C	-6.72	92.85	111.00
4	E	756	LEU	N-CA-C	-6.72	92.87	111.00
4	V	756	LEU	N-CA-C	-6.71	92.89	111.00
3	D	490	TYR	N-CA-C	-6.64	93.08	111.00
3	L	490	TYR	N-CA-C	-6.63	93.10	111.00
6	O	486	ILE	CA-C-N	6.60	135.58	117.10
6	G	486	ILE	CA-C-N	6.58	135.54	117.10
3	L	286	VAL	N-CA-C	-6.53	93.36	111.00
3	D	286	VAL	N-CA-C	-6.52	93.39	111.00
7	P	90	ILE	CA-C-N	6.42	135.08	117.10
7	H	90	ILE	CA-C-N	6.42	135.07	117.10
6	G	792	LEU	N-CA-C	-6.42	93.68	111.00
3	L	461	ILE	N-CA-C	-6.41	93.69	111.00
6	O	792	LEU	N-CA-C	-6.41	93.69	111.00
3	D	461	ILE	N-CA-C	-6.41	93.69	111.00
4	V	254	PHE	N-CA-C	-6.40	93.72	111.00
4	E	254	PHE	N-CA-C	-6.39	93.74	111.00
4	M	254	PHE	N-CA-C	-6.39	93.74	111.00
4	M	324	ALA	N-CA-C	6.32	128.07	111.00
4	V	324	ALA	N-CA-C	6.32	128.05	111.00
5	N	69	TYR	O-C-N	6.31	132.80	122.70
4	E	324	ALA	N-CA-C	6.31	128.04	111.00
3	D	642	GLU	O-C-N	6.30	132.78	122.70
5	W	69	TYR	O-C-N	6.30	132.78	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	69	TYR	O-C-N	6.29	132.77	122.70
3	L	642	GLU	O-C-N	6.29	132.76	122.70
2	K	400	ALA	N-CA-C	-6.26	94.10	111.00
3	L	204	SER	N-CA-C	-6.26	94.10	111.00
3	D	204	SER	N-CA-C	-6.25	94.12	111.00
2	C	400	ALA	N-CA-C	-6.25	94.12	111.00
7	H	66	MET	N-CA-C	-6.22	94.19	111.00
7	P	66	MET	N-CA-C	-6.22	94.21	111.00
3	L	78	ASP	C-N-CA	6.20	137.21	121.70
3	D	196	GLY	CA-C-O	6.20	131.76	120.60
3	D	78	ASP	C-N-CA	6.20	137.19	121.70
3	D	573	LEU	N-CA-C	-6.19	94.29	111.00
3	D	613	ILE	N-CA-C	-6.18	94.31	111.00
3	L	196	GLY	CA-C-O	6.18	131.72	120.60
3	L	573	LEU	N-CA-C	-6.18	94.32	111.00
3	L	613	ILE	N-CA-C	-6.17	94.35	111.00
3	L	469	PHE	N-CA-C	-6.13	94.46	111.00
3	D	469	PHE	N-CA-C	-6.10	94.52	111.00
7	P	56	TYR	N-CA-C	-6.01	94.78	111.00
7	H	56	TYR	N-CA-C	-5.98	94.86	111.00
6	O	376	THR	N-CA-C	-5.91	95.04	111.00
6	G	376	THR	N-CA-C	-5.91	95.05	111.00
2	C	223	GLY	N-CA-C	-5.89	98.38	113.10
4	E	738	ASN	N-CA-C	-5.89	95.11	111.00
2	K	223	GLY	N-CA-C	-5.88	98.40	113.10
4	V	738	ASN	N-CA-C	-5.87	95.16	111.00
4	E	709	LEU	N-CA-C	-5.83	95.26	111.00
4	V	709	LEU	N-CA-C	-5.81	95.31	111.00
5	N	80	ILE	N-CA-C	-5.70	95.62	111.00
2	C	732	HIS	C-N-CA	5.69	135.93	121.70
4	E	759	THR	N-CA-C	-5.69	95.65	111.00
2	K	732	HIS	C-N-CA	5.69	135.92	121.70
5	F	80	ILE	N-CA-C	-5.68	95.65	111.00
2	K	105	TYR	N-CA-C	-5.68	95.65	111.00
4	V	759	THR	N-CA-C	-5.68	95.66	111.00
5	W	80	ILE	N-CA-C	-5.68	95.67	111.00
4	M	550	GLY	C-N-CA	5.67	135.88	121.70
2	C	105	TYR	N-CA-C	-5.67	95.69	111.00
6	G	499	GLU	N-CA-C	5.67	126.30	111.00
4	E	222	GLY	N-CA-C	-5.66	98.96	113.10
4	V	550	GLY	C-N-CA	5.66	135.85	121.70
4	E	550	GLY	C-N-CA	5.66	135.84	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	499	GLU	N-CA-C	5.65	126.25	111.00
4	V	222	GLY	N-CA-C	-5.65	98.98	113.10
3	D	75	GLY	N-CA-C	-5.64	99.00	113.10
3	L	75	GLY	N-CA-C	-5.64	98.99	113.10
4	M	222	GLY	N-CA-C	-5.63	99.01	113.10
3	D	182	GLU	N-CA-C	-5.62	95.83	111.00
3	L	182	GLU	N-CA-C	-5.62	95.83	111.00
2	C	15	LEU	N-CA-C	-5.61	95.86	111.00
6	G	818	ILE	N-CA-C	-5.61	95.86	111.00
4	V	391	PRO	N-CA-C	5.60	126.67	112.10
2	K	15	LEU	N-CA-C	-5.60	95.88	111.00
4	M	391	PRO	N-CA-C	5.59	126.64	112.10
4	E	391	PRO	N-CA-C	5.58	126.61	112.10
6	O	818	ILE	N-CA-C	-5.58	95.93	111.00
6	G	196	MET	N-CA-C	-5.56	95.99	111.00
6	O	503	GLU	N-CA-C	-5.56	96.00	111.00
6	G	503	GLU	N-CA-C	-5.55	96.02	111.00
6	O	196	MET	N-CA-C	-5.53	96.07	111.00
6	O	170	ILE	CA-C-N	5.52	132.55	117.10
3	L	429	GLY	N-CA-C	-5.51	99.32	113.10
6	O	195	MET	N-CA-C	-5.51	96.12	111.00
6	G	195	MET	N-CA-C	-5.51	96.13	111.00
3	D	429	GLY	N-CA-C	-5.50	99.34	113.10
4	V	733	LYS	N-CA-C	-5.50	96.14	111.00
4	E	733	LYS	N-CA-C	-5.50	96.15	111.00
6	G	170	ILE	CA-C-N	5.50	132.50	117.10
7	H	477	ASN	C-N-CA	-5.48	107.99	121.70
4	E	847	LEU	N-CA-C	-5.47	96.22	111.00
2	C	630	GLN	N-CA-C	-5.47	96.22	111.00
2	K	630	GLN	N-CA-C	-5.47	96.23	111.00
5	N	110	GLU	N-CA-C	-5.47	96.23	111.00
5	W	110	GLU	N-CA-C	-5.47	96.24	111.00
4	V	847	LEU	N-CA-C	-5.46	96.25	111.00
5	F	110	GLU	N-CA-C	-5.46	96.26	111.00
3	D	115	LEU	N-CA-C	-5.44	96.32	111.00
3	L	115	LEU	N-CA-C	-5.44	96.32	111.00
6	G	558	ALA	N-CA-C	-5.42	96.37	111.00
4	V	736	ASP	CA-C-O	-5.42	108.73	120.10
2	C	273	ILE	N-CA-C	-5.41	96.40	111.00
2	K	273	ILE	N-CA-C	-5.41	96.41	111.00
6	O	558	ALA	N-CA-C	-5.40	96.43	111.00
4	E	736	ASP	CA-C-O	-5.39	108.77	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	642	GLU	CA-C-O	-5.39	108.77	120.10
2	C	226	ASP	N-CA-C	-5.39	96.44	111.00
4	V	845	ARG	N-CA-C	-5.39	96.45	111.00
4	E	845	ARG	N-CA-C	-5.39	96.46	111.00
3	L	642	GLU	CA-C-O	-5.39	108.79	120.10
2	K	226	ASP	N-CA-C	-5.38	96.48	111.00
4	M	285	LEU	O-C-N	-5.36	114.13	122.70
4	V	285	LEU	O-C-N	-5.36	114.13	122.70
6	G	318	LEU	N-CA-C	5.35	125.44	111.00
6	O	318	LEU	N-CA-C	5.34	125.42	111.00
4	E	285	LEU	O-C-N	-5.34	114.16	122.70
4	E	647	VAL	N-CA-C	-5.33	96.61	111.00
7	P	90	ILE	CA-C-O	-5.33	108.91	120.10
7	H	90	ILE	CA-C-O	-5.33	108.92	120.10
4	V	647	VAL	N-CA-C	-5.32	96.65	111.00
7	H	49	VAL	N-CA-C	-5.30	96.70	111.00
3	D	441	VAL	N-CA-C	-5.29	96.70	111.00
7	P	49	VAL	N-CA-C	-5.29	96.71	111.00
3	L	441	VAL	N-CA-C	-5.28	96.73	111.00
3	D	394	PHE	N-CA-C	-5.22	96.89	111.00
3	L	394	PHE	N-CA-C	-5.21	96.93	111.00
6	G	64	ARG	N-CA-C	5.21	125.06	111.00
6	O	64	ARG	N-CA-C	5.21	125.05	111.00
7	P	19	ARG	C-N-CA	5.20	134.70	121.70
2	C	423	ARG	C-N-CA	5.20	134.69	121.70
2	K	423	ARG	C-N-CA	5.19	134.67	121.70
7	H	19	ARG	C-N-CA	5.19	134.67	121.70
7	H	48	PHE	N-CA-C	-5.18	97.02	111.00
3	L	268	ASN	N-CA-C	-5.17	97.04	111.00
7	P	48	PHE	N-CA-C	-5.17	97.05	111.00
4	V	663	PHE	N-CA-C	-5.16	97.08	111.00
3	D	268	ASN	N-CA-C	-5.15	97.09	111.00
3	L	21	VAL	N-CA-C	-5.15	97.09	111.00
2	C	200	VAL	O-C-N	5.15	130.94	122.70
4	E	663	PHE	N-CA-C	-5.15	97.11	111.00
6	O	775	LEU	N-CA-C	-5.14	97.11	111.00
3	D	21	VAL	N-CA-C	-5.14	97.12	111.00
6	G	169	LEU	N-CA-C	-5.14	97.12	111.00
2	K	200	VAL	O-C-N	5.14	130.93	122.70
6	O	169	LEU	N-CA-C	-5.13	97.14	111.00
6	O	229	GLU	C-N-CA	5.13	134.53	121.70
6	G	229	GLU	C-N-CA	5.13	134.53	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	868	VAL	N-CA-C	-5.13	97.15	111.00
6	G	868	VAL	N-CA-C	-5.12	97.18	111.00
6	G	775	LEU	N-CA-C	-5.11	97.20	111.00
3	D	104	CYS	C-N-CA	5.11	134.47	121.70
3	L	104	CYS	C-N-CA	5.11	134.46	121.70
3	L	543	LEU	O-C-N	-5.09	114.55	122.70
2	K	168	ARG	N-CA-C	-5.08	97.28	111.00
3	D	114	ILE	N-CA-C	-5.08	97.30	111.00
2	C	168	ARG	N-CA-C	-5.07	97.30	111.00
3	L	114	ILE	N-CA-C	-5.07	97.31	111.00
4	M	447	GLU	C-N-CA	5.07	134.37	121.70
6	O	42	LEU	O-C-N	-5.06	114.60	122.70
3	D	543	LEU	O-C-N	-5.06	114.60	122.70
4	V	447	GLU	C-N-CA	5.06	134.35	121.70
6	G	165	ASN	C-N-CA	5.06	134.35	121.70
4	M	248	ASP	O-C-N	-5.06	114.61	122.70
4	E	248	ASP	O-C-N	-5.05	114.62	122.70
2	K	684	GLN	C-N-CA	5.04	132.90	122.30
6	O	165	ASN	C-N-CA	5.04	134.31	121.70
6	O	797	PHE	N-CA-C	-5.04	97.39	111.00
4	E	447	GLU	C-N-CA	5.04	134.30	121.70
4	V	248	ASP	O-C-N	-5.04	114.64	122.70
6	G	797	PHE	N-CA-C	-5.04	97.41	111.00
3	D	20	SER	C-N-CA	5.03	134.28	121.70
6	O	805	LYS	N-CA-C	-5.03	97.41	111.00
3	D	218	ASN	O-C-N	5.03	130.75	122.70
6	G	805	LYS	N-CA-C	-5.03	97.42	111.00
2	C	684	GLN	C-N-CA	5.03	132.86	122.30
3	L	20	SER	C-N-CA	5.03	134.26	121.70
6	G	42	LEU	O-C-N	-5.02	114.67	122.70
2	K	709	ILE	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	317	PHE	Mainchain
2	C	380	CYS	Mainchain
2	C	559	GLY	Mainchain
2	C	63	GLN	Peptide
3	D	119	ASP	Mainchain
3	D	44	HIS	Mainchain

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Mol	Chain	Res	Type	Group
4	E	309	ARG	Peptide
4	E	323	THR	Peptide
4	E	442	PHE	Peptide
4	E	447	GLU	Peptide
5	F	59	ILE	Mainchain
6	G	235	CYS	Peptide
6	G	254	GLN	Peptide
6	G	274	ALA	Peptide
6	G	309	LYS	Peptide
6	G	311	HIS	Peptide
6	G	329	LEU	Peptide
6	G	331	THR	Peptide
6	G	348	VAL	Peptide
6	G	471	ASP	Peptide
6	G	499	GLU	Mainchain
6	G	581	PHE	Peptide
6	G	65	PHE	Mainchain
6	G	897	LYS	Peptide
6	G	91	ASP	Mainchain
2	K	317	PHE	Mainchain
2	K	380	CYS	Mainchain
2	K	559	GLY	Mainchain
2	K	63	GLN	Peptide
3	L	119	ASP	Mainchain
3	L	44	HIS	Mainchain
4	M	309	ARG	Peptide
4	M	323	THR	Peptide
4	M	442	PHE	Peptide
4	M	447	GLU	Peptide
5	N	59	ILE	Mainchain
6	O	235	CYS	Peptide
6	O	254	GLN	Peptide
6	O	274	ALA	Peptide
6	O	309	LYS	Peptide
6	O	311	HIS	Peptide
6	O	329	LEU	Peptide
6	O	331	THR	Peptide
6	O	348	VAL	Peptide
6	O	471	ASP	Peptide
6	O	499	GLU	Mainchain
6	O	581	PHE	Peptide
6	O	65	PHE	Mainchain

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Mol	Chain	Res	Type	Group
6	O	897	LYS	Peptide
6	O	91	ASP	Mainchain
4	V	309	ARG	Peptide
4	V	323	THR	Peptide
4	V	442	PHE	Peptide
4	V	447	GLU	Peptide
5	W	59	ILE	Mainchain

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	636	0	181	0	0
1	B	636	0	181	0	0
1	I	636	0	181	0	0
1	J	636	0	181	2	0
1	R	636	0	181	0	0
2	C	4503	0	1194	3	0
2	K	4503	0	1194	0	0
3	D	3211	0	880	2	0
3	L	3211	0	880	17	0
4	E	3294	0	852	1	0
4	M	2199	0	570	1	0
4	V	3294	0	852	18	0
5	F	555	0	148	0	0
5	N	555	0	148	0	0
5	W	555	0	148	0	0
6	G	3250	0	833	0	0
6	O	3250	0	833	0	0
7	H	1520	0	406	3	0
7	P	539	0	142	0	0
8	X	1169	0	303	0	0
8	Z	1169	0	303	0	0
All	All	39957	0	10591	28	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:349:GLY:HA2	4:V:206:ASN:C	1.53	1.27
3:L:349:GLY:HA2	4:V:206:ASN:O	1.39	1.18
3:L:350:SER:H	4:V:207:ASP:N	1.42	1.16
3:L:350:SER:H	4:V:207:ASP:CA	1.58	1.14
3:L:351:CYS:N	4:V:210:ALA:CA	2.24	1.01
3:D:270:GLY:HA3	1:J:137:ALA:CA	1.95	0.97
3:L:349:GLY:CA	4:V:206:ASN:O	2.12	0.97
3:L:349:GLY:CA	4:V:206:ASN:C	2.34	0.96
3:L:350:SER:N	4:V:207:ASP:N	2.17	0.93
2:C:607:LYS:CA	2:C:1130:GLU:O	2.18	0.92
3:L:351:CYS:H	4:V:210:ALA:CA	1.81	0.89
3:L:350:SER:N	4:V:207:ASP:CA	2.38	0.85
7:H:296:GLU:CA	7:H:368:THR:H	1.95	0.79
3:L:350:SER:CA	4:V:210:ALA:H	2.01	0.73
7:H:356:ASN:CA	7:H:362:LEU:H	2.10	0.65
3:L:351:CYS:N	4:V:210:ALA:N	2.46	0.64
3:L:349:GLY:CA	4:V:207:ASP:N	2.75	0.48
2:C:608:TYR:N	2:C:1130:GLU:O	2.47	0.48
2:C:607:LYS:CA	2:C:1130:GLU:C	2.85	0.45
7:H:356:ASN:C	7:H:362:LEU:H	2.20	0.45
3:L:349:GLY:HA2	4:V:206:ASN:CA	2.43	0.45
3:L:350:SER:C	4:V:210:ALA:H	2.19	0.45
3:L:376:ILE:CA	4:V:245:GLY:HA2	2.47	0.44
3:L:350:SER:C	4:V:210:ALA:N	2.72	0.43
3:D:270:GLY:CA	1:J:137:ALA:CA	2.82	0.43
4:E:249:SER:C	4:E:251:LEU:H	2.23	0.42
4:V:249:SER:C	4:V:251:LEU:H	2.23	0.42
4:M:249:SER:C	4:M:251:LEU:H	2.23	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	157/181 (87%)	153 (98%)	4 (2%)	0	100 100
1	B	157/181 (87%)	153 (98%)	4 (2%)	0	100 100
1	I	157/181 (87%)	153 (98%)	4 (2%)	0	100 100
1	J	157/181 (87%)	153 (98%)	4 (2%)	0	100 100
1	R	157/181 (87%)	153 (98%)	4 (2%)	0	100 100
2	C	1122/1262 (89%)	972 (87%)	104 (9%)	46 (4%)	3 23
2	K	1122/1262 (89%)	972 (87%)	104 (9%)	46 (4%)	3 23
3	D	801/905 (88%)	700 (87%)	64 (8%)	37 (5%)	2 21
3	L	801/905 (88%)	701 (88%)	63 (8%)	37 (5%)	2 21
4	E	820/874 (94%)	749 (91%)	40 (5%)	31 (4%)	3 24
4	M	548/874 (63%)	492 (90%)	27 (5%)	29 (5%)	2 19
4	V	820/874 (94%)	749 (91%)	40 (5%)	31 (4%)	3 24
5	F	137/177 (77%)	128 (93%)	7 (5%)	2 (2%)	10 46
5	N	137/177 (77%)	128 (93%)	7 (5%)	2 (2%)	10 46
5	W	137/177 (77%)	128 (93%)	7 (5%)	2 (2%)	10 46
6	G	809/968 (84%)	658 (81%)	84 (10%)	67 (8%)	1 12
6	O	809/968 (84%)	658 (81%)	84 (10%)	67 (8%)	1 12
7	H	376/511 (74%)	336 (89%)	31 (8%)	9 (2%)	6 33
7	P	133/511 (26%)	116 (87%)	16 (12%)	1 (1%)	19 60
8	X	290/308 (94%)	276 (95%)	9 (3%)	5 (2%)	9 42
8	Z	290/308 (94%)	276 (95%)	10 (3%)	4 (1%)	11 46
All	All	9937/11966 (83%)	8804 (89%)	717 (7%)	416 (4%)	5 22

All (416) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	11	ARG
2	C	227	ARG
2	C	526	GLU
2	C	572	ARG
2	C	686	ASN
2	C	949	VAL
2	C	999	VAL
3	D	6	ASP
3	D	284	ASN
3	D	329	ALA

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Mol	Chain	Res	Type
3	D	336	LYS
3	D	350	SER
3	D	484	SER
3	D	513	ALA
3	D	615	LYS
3	D	791	PRO
3	D	795	GLU
4	E	117	GLU
4	E	280	CYS
4	E	309	ARG
4	E	323	THR
4	E	324	ALA
4	E	391	PRO
4	E	393	LYS
4	E	413	TYR
4	E	448	PHE
4	E	549	ASN
5	F	36	PRO
6	G	55	LEU
6	G	69	LEU
6	G	85	VAL
6	G	90	PRO
6	G	173	ALA
6	G	181	LEU
6	G	197	LEU
6	G	237	ALA
6	G	253	LEU
6	G	275	PRO
6	G	331	THR
6	G	499	GLU
6	G	506	ILE
6	G	508	VAL
6	G	523	THR
6	G	543	ARG
6	G	770	ASN
6	G	785	GLU
6	G	792	LEU
6	G	814	ILE
6	G	826	ALA
6	G	939	THR
6	G	959	ILE
7	H	326	GLN

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Mol	Chain	Res	Type
7	H	361	VAL
2	K	11	ARG
2	K	227	ARG
2	K	526	GLU
2	K	572	ARG
2	K	686	ASN
2	K	949	VAL
2	K	999	VAL
3	L	6	ASP
3	L	284	ASN
3	L	329	ALA
3	L	336	LYS
3	L	350	SER
3	L	484	SER
3	L	513	ALA
3	L	615	LYS
3	L	791	PRO
3	L	795	GLU
4	M	117	GLU
4	M	280	CYS
4	M	309	ARG
4	M	323	THR
4	M	324	ALA
4	M	391	PRO
4	M	393	LYS
4	M	413	TYR
4	M	448	PHE
4	M	549	ASN
5	N	36	PRO
6	O	55	LEU
6	O	69	LEU
6	O	85	VAL
6	O	90	PRO
6	O	173	ALA
6	O	181	LEU
6	O	197	LEU
6	O	237	ALA
6	O	253	LEU
6	O	275	PRO
6	O	331	THR
6	O	499	GLU
6	O	506	ILE

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Mol	Chain	Res	Type
6	O	508	VAL
6	O	523	THR
6	O	543	ARG
6	O	770	ASN
6	O	785	GLU
6	O	792	LEU
6	O	814	ILE
6	O	826	ALA
6	O	939	THR
6	O	959	ILE
4	V	117	GLU
4	V	280	CYS
4	V	309	ARG
4	V	323	THR
4	V	324	ALA
4	V	391	PRO
4	V	393	LYS
4	V	413	TYR
4	V	448	PHE
4	V	549	ASN
5	W	36	PRO
8	X	111	SER
8	X	231	ARG
8	Z	111	SER
8	Z	231	ARG
2	C	137	TYR
2	C	226	ASP
2	C	425	ARG
2	C	441	LYS
2	C	498	ALA
2	C	538	SER
2	C	546	SER
2	C	621	VAL
2	C	642	VAL
2	C	1178	ARG
3	D	17	ARG
3	D	59	PRO
3	D	273	ARG
3	D	410	SER
3	D	426	PRO
3	D	630	PHE
3	D	739	ASP

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Mol	Chain	Res	Type
4	E	263	HIS
4	E	310	THR
4	E	313	LYS
4	E	373	ASP
4	E	442	PHE
4	E	484	HIS
4	E	551	LEU
4	E	739	THR
4	E	741	GLU
6	G	83	GLU
6	G	103	ASP
6	G	174	PRO
6	G	307	GLU
6	G	554	ALA
6	G	558	ALA
6	G	879	ASP
7	H	351	LYS
2	K	137	TYR
2	K	226	ASP
2	K	337	LYS
2	K	425	ARG
2	K	441	LYS
2	K	498	ALA
2	K	538	SER
2	K	546	SER
2	K	621	VAL
2	K	630	GLN
2	K	642	VAL
2	K	1178	ARG
3	L	17	ARG
3	L	59	PRO
3	L	273	ARG
3	L	410	SER
3	L	426	PRO
3	L	630	PHE
3	L	739	ASP
4	M	263	HIS
4	M	310	THR
4	M	313	LYS
4	M	373	ASP
4	M	442	PHE
4	M	484	HIS

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Mol	Chain	Res	Type
4	M	551	LEU
6	O	83	GLU
6	O	103	ASP
6	O	174	PRO
6	O	307	GLU
6	O	554	ALA
6	O	558	ALA
6	O	879	ASP
4	V	263	HIS
4	V	310	THR
4	V	313	LYS
4	V	373	ASP
4	V	442	PHE
4	V	484	HIS
4	V	551	LEU
4	V	739	THR
4	V	741	GLU
2	C	205	ASP
2	C	337	LYS
2	C	345	ASP
2	C	348	SER
2	C	349	SER
2	C	387	GLU
2	C	469	ALA
2	C	594	PRO
2	C	619	LYS
2	C	624	SER
2	C	627	ALA
2	C	630	GLN
2	C	790	PRO
3	D	140	GLY
3	D	260	THR
3	D	272	GLU
3	D	571	ASN
3	D	601	ARG
3	D	662	VAL
3	D	694	GLN
3	D	735	GLN
4	E	256	GLU
4	E	353	SER
4	E	522	ASN
4	E	569	PRO

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Mol	Chain	Res	Type
5	F	55	THR
6	G	18	SER
6	G	22	SER
6	G	194	PHE
6	G	257	SER
6	G	259	ALA
6	G	308	LEU
6	G	318	LEU
6	G	487	PRO
6	G	501	LYS
6	G	528	SER
6	G	817	ASN
6	G	904	GLY
7	H	45	GLN
7	H	358	ASP
7	H	398	GLN
7	H	447	ALA
2	K	205	ASP
2	K	345	ASP
2	K	348	SER
2	K	349	SER
2	K	387	GLU
2	K	469	ALA
2	K	594	PRO
2	K	619	LYS
2	K	624	SER
2	K	627	ALA
2	K	790	PRO
3	L	140	GLY
3	L	260	THR
3	L	272	GLU
3	L	571	ASN
3	L	601	ARG
3	L	662	VAL
3	L	694	GLN
3	L	735	GLN
4	M	256	GLU
4	M	353	SER
4	M	522	ASN
4	M	569	PRO
5	N	55	THR
6	O	18	SER

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Mol	Chain	Res	Type
6	O	22	SER
6	O	194	PHE
6	O	257	SER
6	O	259	ALA
6	O	308	LEU
6	O	318	LEU
6	O	487	PRO
6	O	501	LYS
6	O	528	SER
6	O	817	ASN
6	O	904	GLY
7	P	45	GLN
4	V	256	GLU
4	V	353	SER
4	V	522	ASN
4	V	569	PRO
5	W	55	THR
2	C	133	GLY
2	C	193	THR
2	C	271	LYS
2	C	423	ARG
2	C	452	ASN
2	C	731	GLY
3	D	89	LEU
3	D	318	LYS
3	D	734	LEU
3	D	740	ALA
3	D	787	SER
3	D	788	LEU
4	E	40	ASN
4	E	251	LEU
4	E	464	PRO
6	G	332	PRO
6	G	446	PHE
6	G	537	GLU
6	G	583	ALA
6	G	876	ASP
6	G	916	PHE
7	H	309	LYS
7	H	359	VAL
2	K	133	GLY
2	K	193	THR

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Mol	Chain	Res	Type
2	K	271	LYS
2	K	423	ARG
2	K	452	ASN
2	K	731	GLY
3	L	89	LEU
3	L	318	LYS
3	L	577	ASP
3	L	734	LEU
3	L	740	ALA
3	L	787	SER
3	L	788	LEU
4	M	40	ASN
4	M	251	LEU
4	M	464	PRO
6	O	332	PRO
6	O	446	PHE
6	O	537	GLU
6	O	583	ALA
6	O	876	ASP
6	O	916	PHE
4	V	40	ASN
4	V	251	LEU
4	V	464	PRO
8	X	113	ASP
8	Z	113	ASP
2	C	470	ASP
2	C	698	LYS
2	C	793	LYS
2	C	812	THR
3	D	577	ASP
4	E	221	HIS
4	E	311	LEU
4	E	410	GLY
6	G	32	LYS
6	G	99	ILE
6	G	262	TYR
6	G	330	SER
6	G	372	GLU
6	G	794	PRO
6	G	894	THR
6	G	898	ALA
6	G	900	SER

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Mol	Chain	Res	Type
6	G	962	SER
2	K	470	ASP
2	K	698	LYS
2	K	793	LYS
2	K	812	THR
4	M	221	HIS
4	M	311	LEU
4	M	410	GLY
6	O	32	LYS
6	O	99	ILE
6	O	262	TYR
6	O	330	SER
6	O	372	GLU
6	O	794	PRO
6	O	894	THR
6	O	898	ALA
6	O	900	SER
6	O	962	SER
4	V	221	HIS
4	V	311	LEU
4	V	410	GLY
2	C	442	ASN
2	C	781	GLU
3	D	391	ALA
6	G	21	PRO
6	G	102	CYS
6	G	230	LEU
6	G	503	GLU
2	K	442	ASN
2	K	781	GLU
3	L	391	ALA
6	O	21	PRO
6	O	102	CYS
6	O	230	LEU
6	O	503	GLU
3	D	790	ASP
6	G	216	VAL
6	G	238	ASN
3	L	790	ASP
6	O	216	VAL
6	O	238	ASN
2	C	780	PRO

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Continued from previous page...

Mol	Chain	Res	Type
2	C	799	ALA
3	D	355	PRO
6	G	540	PRO
2	K	780	PRO
2	K	799	ALA
3	L	355	PRO
6	O	540	PRO
8	X	213	SER
8	Z	213	SER
3	D	762	LEU
4	E	278	PRO
6	G	531	ARG
3	L	762	LEU
4	M	278	PRO
6	O	531	ARG
4	V	278	PRO
3	D	200	PRO
4	E	556	PRO
6	G	317	VAL
3	L	200	PRO
4	M	556	PRO
6	O	317	VAL
4	V	556	PRO
2	C	247	GLY
2	C	488	ILE
2	K	247	GLY
2	K	488	ILE
8	X	45	SER

5.3.2 Protein sidechains [\(i\)](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

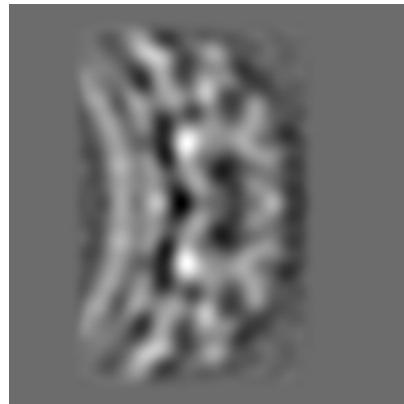
6 Tomogram visualisation [\(i\)](#)

This section contains visualisations of the EMDB entry EMD-2989. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

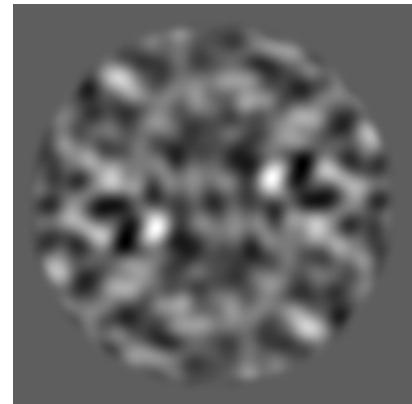
6.1 Orthogonal projections [\(i\)](#)



X



Y



Z

The images above show the tomogram projected in three orthogonal directions.

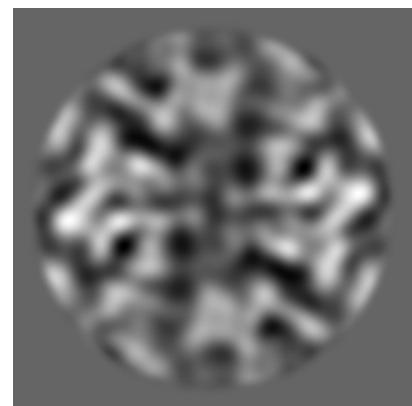
6.2 Central slices [\(i\)](#)



X Index: 100



Y Index: 100



Z Index: 100

The images above show central slices of the tomogram in three orthogonal directions.

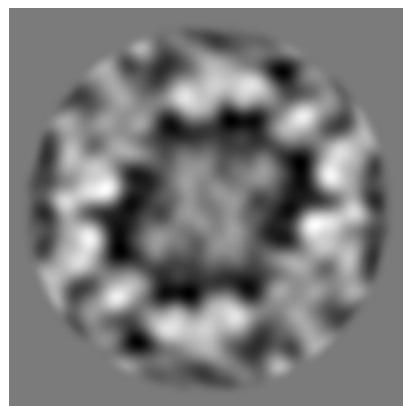
6.3 Largest variance slices [\(i\)](#)



X Index: 70



Y Index: 108



Z Index: 78

The images above show the largest variance slices of the tomogram in three orthogonal directions.

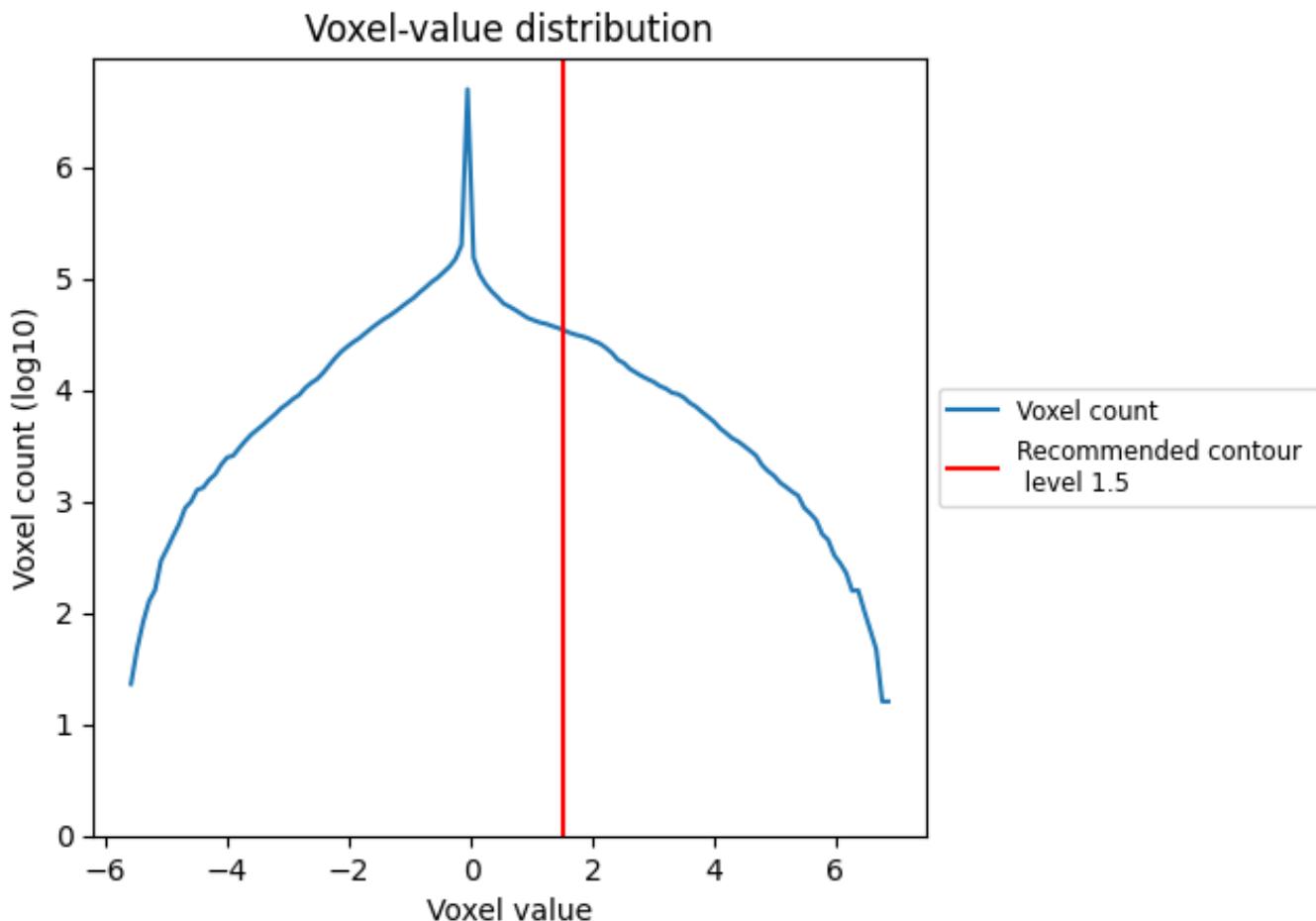
6.4 Mask visualisation [\(i\)](#)

This section was not generated. No masks/segmentation were deposited.

7 Tomogram analysis (i)

This section contains the results of statistical analysis of the tomogram.

7.1 Voxel-value distribution (i)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

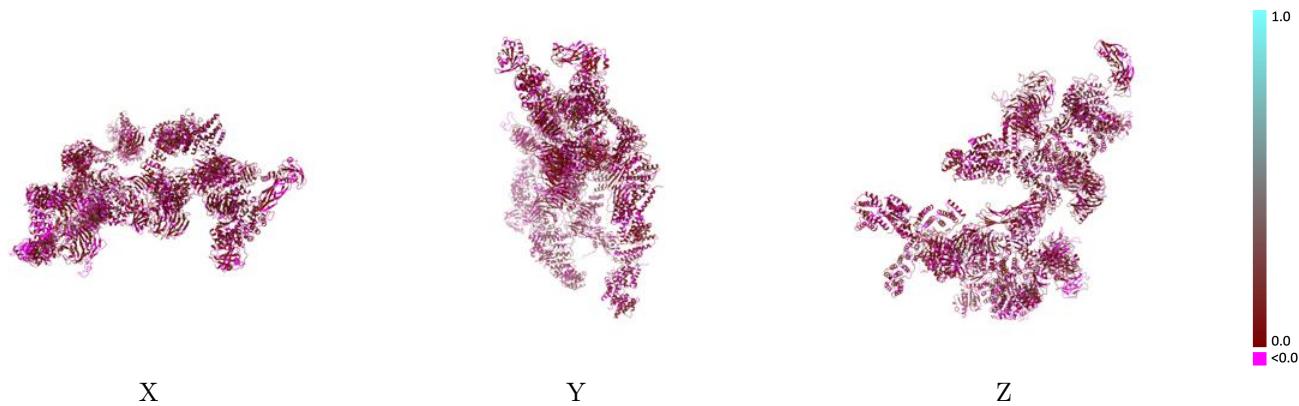
8 Map-model fit [\(i\)](#)

This section contains information regarding the fit between EMDB map EMD-2989 and PDB model 5A1Y. Per-residue inclusion information can be found in section 3 on page 9.

8.1 Map-model overlay [\(i\)](#)

This section was not generated.

8.2 Q-score mapped to coordinate model [\(i\)](#)

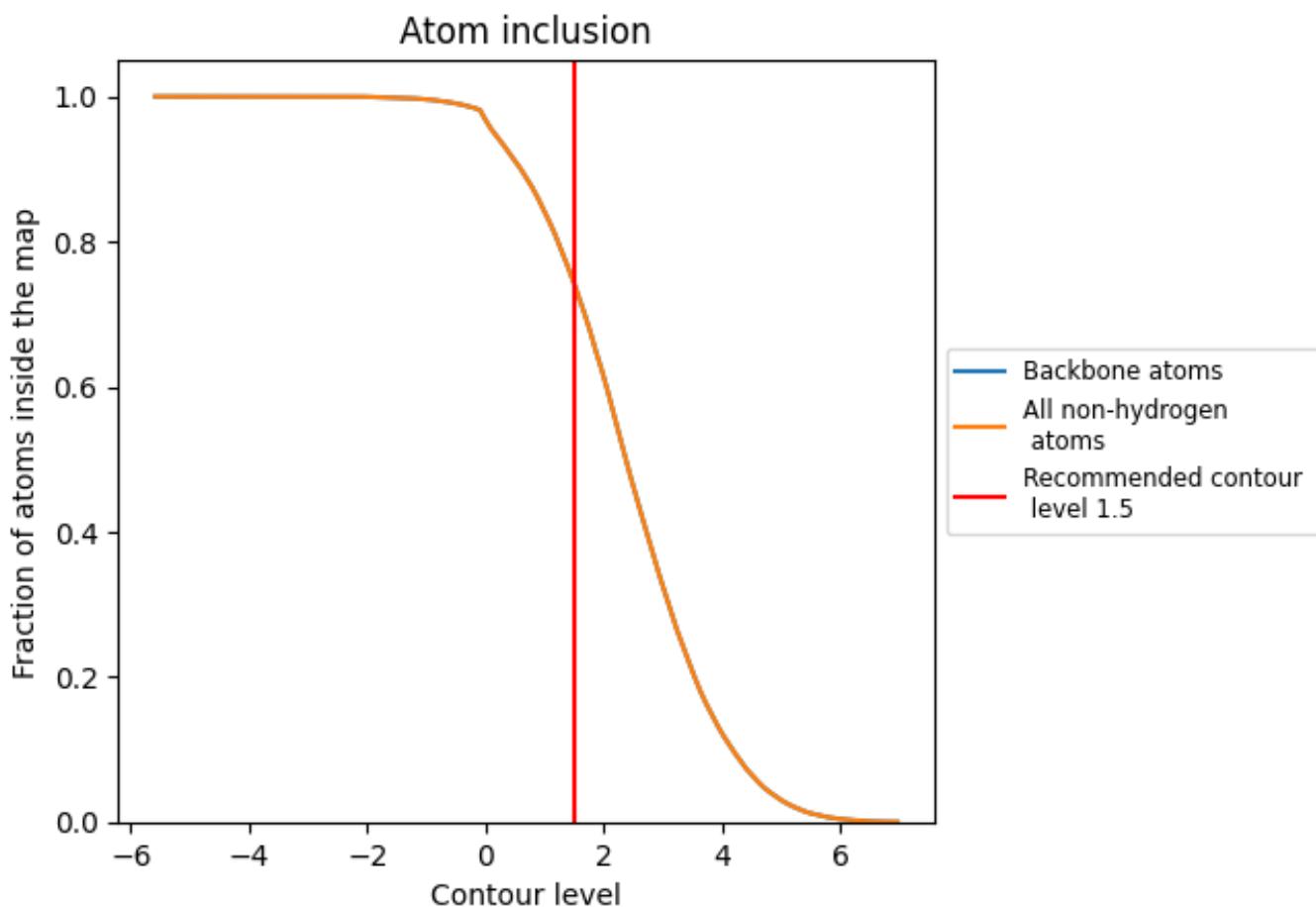


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model [\(i\)](#)

This section was not generated.

8.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 74% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary [\(i\)](#)

The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7414	0.0600
A	0.6965	0.0490
B	0.8899	0.0590
C	0.8899	0.0680
D	0.8708	0.0730
E	0.7790	0.0660
F	0.7856	0.0710
G	0.8631	0.0710
H	0.7164	0.0640
I	0.2280	0.0330
J	0.4827	0.0500
K	0.6960	0.0530
L	0.8184	0.0690
M	0.3997	0.0220
N	0.5279	0.0670
O	0.5502	0.0470
P	0.7737	0.0440
R	0.6887	0.0540
V	0.7413	0.0680
W	0.8306	0.0590
X	0.9153	0.0690
Z	0.7819	0.0490

